CA3 ONHW Q90
82 U6506 v.2

Air quality surveys of Upper Ottawa Street Landfill Site - final report
Reference 14

Digitized by the Internet Archive
in 2024 with funding from
Hamilton Public Library

https://archive.org/details/airqualitysurvey02unse

HAMILTON PUBLIC LIBRARY

APR 3 - 1987

COPY

URBAN MUNICIPAL

MAY 4 1987

GOVERNMENT DOCUMENTS

Reference # 14

FINAL REPORT

AIR QUALITY SURVEYS
OF
UPPER OTTAWA STREET LANDFILL SITE

Prepared For:
UPPER OTTAWA STREET LANDFILL STUDY,
42 JAMES STREET SOUTH, SUITE 33,
HAMILTON, ONTARIO L8P 2Y4

Prepared By:
SCIEX
Division of MDS HEALTH GROUP LIMITED,
55 Glen Cameron Road, Suite 202,
Thornhill, Ontario L3T 1P2

REFERENCE 5

January 1983

TABLE OF CONTENTS

		Page
1.0	SUMMARY AND CONCLUSIONS	1
2.0	INTRODUCTION	6
2.1	GENERAL	6
2.2	WORK PROGRAM	13
3.0	DISCRETE SAMPLE ANALYSIS BY MS/MS	15
3.1	GENERAL	15
3.2	SAMPLE ANALYSIS	15
3.3	RESULTS	15
4.0	CONCENTRATION ESTIMATES OF PRIORITY CHEMICALS FOR 1981 SURVEY	20
5.0	COMPARATIVE FIELD STUDIES	22
5.1	GENERAL	22
5.2	UPPER OTTAWA STREET LANDFILL/ ANCASTER LANDFILL	22
5.3	RESIDENTIAL AREA COMPARISON	22
6.0	CHLORINATED HYDROCARBON SURVEY	25
6.1	GENERAL	25
6.2	RESULTS	25

LIST OF TABLES

		Page
1.0-1	Summary of Quantitative Results for the Confirmed Chemicals and Carbaryl	5
2.1-1	Summary of Sampling Sites and Dates	7
4.0-1	Concentration Estimates for Confirmed Chemicals (1981 Survey)	21
5.2-1	Upper Ottawa/Ancaster - Sampling Date, June 30, 1982	23
5.3-1	Hamilton - Sampling Date - June 30, 1982	24

LIST OF FIGURES

2.1-1	Approximate Locations of the Sampling Sites	8
2.1-2	Selective Monitoring of Volatile Pollutants	10
2.1-3	Schematic Representation of the Similarities Between GC/MS and MS/MS Analytical Techniques	12
3.3-1	CID Spectra of m/z 94 in Air Bag and o-, m-, and p- methylpyridine	18
6.2-1	Background Van Air Using DASCI After Vent 1, HI RE/RO	26
6.2-2	Site 7: Sampling Vent 4A Using DASCI Source, HI RE/RO	27
6.2-3	Scan of Bag Content from Hamilton Dump Minus Background	28

LIST OF APPENDICES

1. Analysis Methodology Using the TAGA System
2. Chemicals Tentatively Identified Using the Mobile TAGA 3000 Single MS System
3. Profile of Detected Chemicals, Uses, Toxicity and TLV's
4. TAGA Calibration

1.0 SUMMARY AND CONCLUSIONS

This report is the result of extended air quality studies in the Upper Ottawa Street Landfill site, Hamilton, Ontario. The total program consisted of:

a) Air quality field surveys conducted on August 19, 20, 21, and November 5, 1981. These surveys consisted of discrete sample analysis and realtime monitoring using the mobile TAGA 3000 single mass spectrometer. Discrete samples were collected from vents 1 and 2 using both passive badge monitors:

(Dupont; Pro-Tech; activated charcoal) and sorbent tubes (Florisil and charcoal). The samples and sorbent tubes were analyzed by Wellington Environmental Consultants Inc., Guelph, Ontario using capillary column GC with an electron capture detector. It was found that:

i) No PCBs were detected above 0.1 $\mu g/m^3$.

ii) The air extracts were analyzed for 12 common chlorinated pesticides (including Mirex). Of these, only lindane was detected and its level was very close to the detection limit of less than 0.1 $\mu g/m^3$.

iii) Chlorinated benzenes were detected in trace levels close to the detection limits of GC/ECD 0.1 $\mu g/m^3$.

The realtime monitoring using the TAGA 3000 consisted of direct analysis of gas vents, off-site monitoring in the residential areas and the general landfill surface. These results showed a complex mixture of chemicals emanating from the site. Tentative identification of the detected chemicals was proposed using the molecular weight assignment of mixture components, selective chemical ionization methodology, and thermochemical properties of chemical structures.

Based on a toxicity assessment (by FDC Consultants Inc.) of the preliminary lists of detected chemicals, a short priority list of chemicals was selected for further study.

b) The priority list chosen by FDC and the Study Group consists of four general classes as follows:

Proven Carcinogens (First Priority)

benzidine
dimethyl nitrosamine
ethylenimine
8-hydroxy quinoline
1-, 2- naphthylamine
xylenol
phenol

Reproductive Toxins (Second Priority)

acetaminophen
butyl acrylate
acrylic acid
thiocyanic acid

Indefinite Carcinogens (Third Priority)

acrolein
aniline (methyl pyridine)
cresols
diphenylamine
hydroquinone
maleic anhydride
maleic hydrazide
quinone
sorbic acid
styrene
urethane

Potential Nitrosation Substrates (Fourth Priority)

dimethylamine
cyclohexylamine
carbofuran
bufencarb
carbaryl
nitrosodiphenylamine
nitrosophenol
tributylamine
triethanolamine

c) Further investigation of this priority list consisted of detailed analysis of air bag samples collected from the Upper Ottawa Street Landfill and Ancaster Municipal Landfill. The analysis technique used in this study utilized direct analysis of the collected air samples on a sequential mass spectrometer (TAGA 6000 MS/MS). Detailed analysis of the mass spectra of the priority chemical standards was compared to the corresponding peaks in the air bags. Theresults of this analysis can be broken qualitatively into confirmed identities, unconfirmed identities and insufficient information.

The unconfirmed chemicals (that is the pure priority standards did not correspond to the detected peaks in the air bags) are:

Proven Carcinogens

benzidine
dimethyl nitrosamine
ethylenimine
8- hydroxyquinoline
1-,2- naphthylamine

Reproductive Toxins

acetaminophen
butyl acrylate
thiocyanic acid

Indefinite Carcinogens

acrolein
aniline
diphenylamine
hydroquinone
maleic anhydride
maleic hydrazide
quinone
sorbic acid
styrene
urethane

Potential Nitrosation Products

dimethylamine
cyclohexylamine
carbofuran
bufencarb
nitrosodiphenylamine
nitrosophenol
tributylamine
triethanolamine

Alternate assignments of the unconfirmed chemicals were formulated based on the fundamental mass spectra of chemicals. Of the alternate assignments only one chemical: methylpyridine (alternate to aniline) was considered potentially toxic. This chemical was subsequently acquired and confirmed as a component in the air bag samples.

Hence, the confirmed chemicals are:

methylpyridine
acrylic acid
phenol
cresol
xylenol

Inconclusive evidence was found for carbaryl due to its low abundance in the air bag samples. This chemical will be assumed to exist as a worst case possibility and the corresponding concentration will be assumed to be due to carbaryl.

d) Quantitation and comparative studies were conducted for sampling locations near the Upper Ottawa Street Landfill and the Ancaster Municipal Landfill as well as the residential area of Upper Ottawa Street and the residential areas of Hamilton. Table 1.0-1 shows the total results for 1981 surveys and 1982 surveys.

The results show:

i) Very low concentrations for the five chemicals.

ii) No significant differences exist between the residential areas surrounding the landfill sites (Upper Ottawa and Ancaster).

iii) The comparative studies of the residential area around Upper Ottawa and Hamilton show that the two industrial sites, Burlington and Stapleton, and Gage and King, show higher concentrations of the chemicals than the Upper Ottawa Street or the control areas (Chester, Mahony Park).

e) A chlorinated hydrocarbon survey was conducted on August 13, 1982 at Vents 1 and 4A of Upper Ottawa Street Landfill, Blessed Kateri School and Sterling School using a modified TAGA 3000 specially adapted for chlorinated hydrocarbon detection and monitoring. No chlorinated hydrocarbons were detected above the detection limits of 1 ppb.

Detailed information on all of the above programs are included in this report.

TABLE 1

SUMMARY OF QUANTITATIVE RESULTS FOR THE CONFIRMED CHEMICALS AND CARBARYL

* All Concentrations are in parts-per-billion (ppb)

Sampling Site	Methylpyridine	Carbaryl	Acrylic Acid	Phenol	Cresol	Xylenol
Threshold Limit Value (TLV)	5 ppm	5 ppm	No Data	5 ppm	5 ppm	No Data
(A) 1981 Survey:						
Tekawitha School	0.010	0.002	1.22	0.15	0.001	0.50
10 meters from Landfill Gate	0.008	0.001	1.37	0.04	0.001	0.35
Lime Ridge Road	0.016	0.018	3.49	0.15	0.005	1.11
Stone Church and Upper Ottawa	0.024	0.015	4.72	0.23	0.007	1.25
Arbur Street	0.011	0.014	3.16	0.11	0.004	0.95
(B) June 30, 1982 Survey:						
i) Upper Ottawa Landfill -						
Upwind Near Lime Ridge and Upper Kenilworth	0.22	0.00	0.74	0.15	0.004	0.40
Downwind (NE) From Stone Church	0.12	0.07	0.87	0.10	0.003	0.34
ii) Ancaster Landfill -						
Upwind Near Hwy. 2 and Shavers St.	0.07	0.00	0.38	0.08	0.003	0.26
Downwind at Gate (SE-SW)	0.09	0.05	0.43	0.05	0.00	0.25
(C) Comparative Residential Area Studies:						
Stone Church (by the Reservoir)	0.10	0.00	0.80	0.07	0.003	0.65
King Ridge Plaza on Lime Ridge Rd.	0.12	0.00	0.42	0.06	0.002	0.46
Chester Avenue	0.01	0.03	0.68	0.22	0.003	0.94
Burlington & Stapleton	3.17	0.20	3.60	1.29	0.017	1.94
Mahony Park	0.00	0.00	0.00	0.00	0.00	0.00
Ottawa/Parkdale/Marton/Burlington	0.01	0.00	0.00	0.33	0.00	0.00
Hamilton Downtown (Gage & King)	0.63	0.10	2.22	1.28	0.29	44.54

2.0 INTRODUCTION

2.1 GENERAL

The SCIEX Division of MDS Health Group Limited was contracted by the Upper Ottawa Street Landfill Study to conduct air quality surveys at the Upper Ottawa Street Landfill (UOSL) in Hamilton, Ontario.

The overall objectives of the 1981 program were:

a) To qualitatively identify as many pollutants as possible emanating from the UOSL site.

b) To compare the "air quality", in terms of pollutant types, on UOSL to air quality upwind and downwind of the site. This will enable the UOSL Study Group to determine whether or not the landfill is contributing any air pollutants to the general background in Hamilton.

In order to achieve the above objectives, field surveys were conducted on August 19, 20, 21 and November 5, 1981. The sampling program consisted of discrete samples and realtime monitoring on location using the mobile Trace Atmospheric Gas Analyzer (TAGA 3000). A summary of sampling sites and dates is shown in Table 2.1-1. The approximate locations of the sampling sites are shown in Figure 2.1-1.

In February 1982, we submitted a report detailing the preliminary identification of chemicals detected within the vents and on the residential sites. Appendix 1 is included to assist in understanding the advantages and limitations of the technique used in 1981.

The results showed that a large number of chemicals exist on the site. These chemicals were vented into ambient air at very small flow rates and volumes. Appendix 2 shows the lists of chemical compounds detected in the vents and on the residential sites. In order to appreciate the significance of the 1981 results, it is important to highlight the following:

a) The mobile TAGA 3000 is a single mass spectrometric technique where ambient air/vented gases are directly sampled and analyzed.

b) The observed measurement is in ion intensity for a given mass-to-charge (m/z).

c) Each m/z can be correlated to the Molecular Weight (MW) of a chemical as follows:

i) positive ion mode: $m/z = MW+1$

ii) negative ion mode: $m/z = MW-1$

iii) charge transfer spectra for both positive and negative ion modes: $m/z = MW$

TABLE 2.1-1

SUMMARY OF SAMPLING SITES AND DATES

Date	Location
August 19	Inner Gate of Landfill Site
	Tekokwitha School
	Vent #4 (opposite Arbur Street)
	Vent #3 (opposite Arbur Street)
	Vent #2 (opposite Stone Church Road)
	Vent #1 (opposite Stone Church Road)
August 20	Vent #0 (opposite Ottawa Street)
	Vent #1
	Vent #2
August 21	Lime Ridge Road (Solomone Street)
	Stone Church and Upper Ottawa Street, Arbur Street
November 5	Vent #2A (old solidification site)
	Vent #2B (old solidification site)
	Vent #4A (same as 4, new core)
	Vent #4B (same as 4, new core)

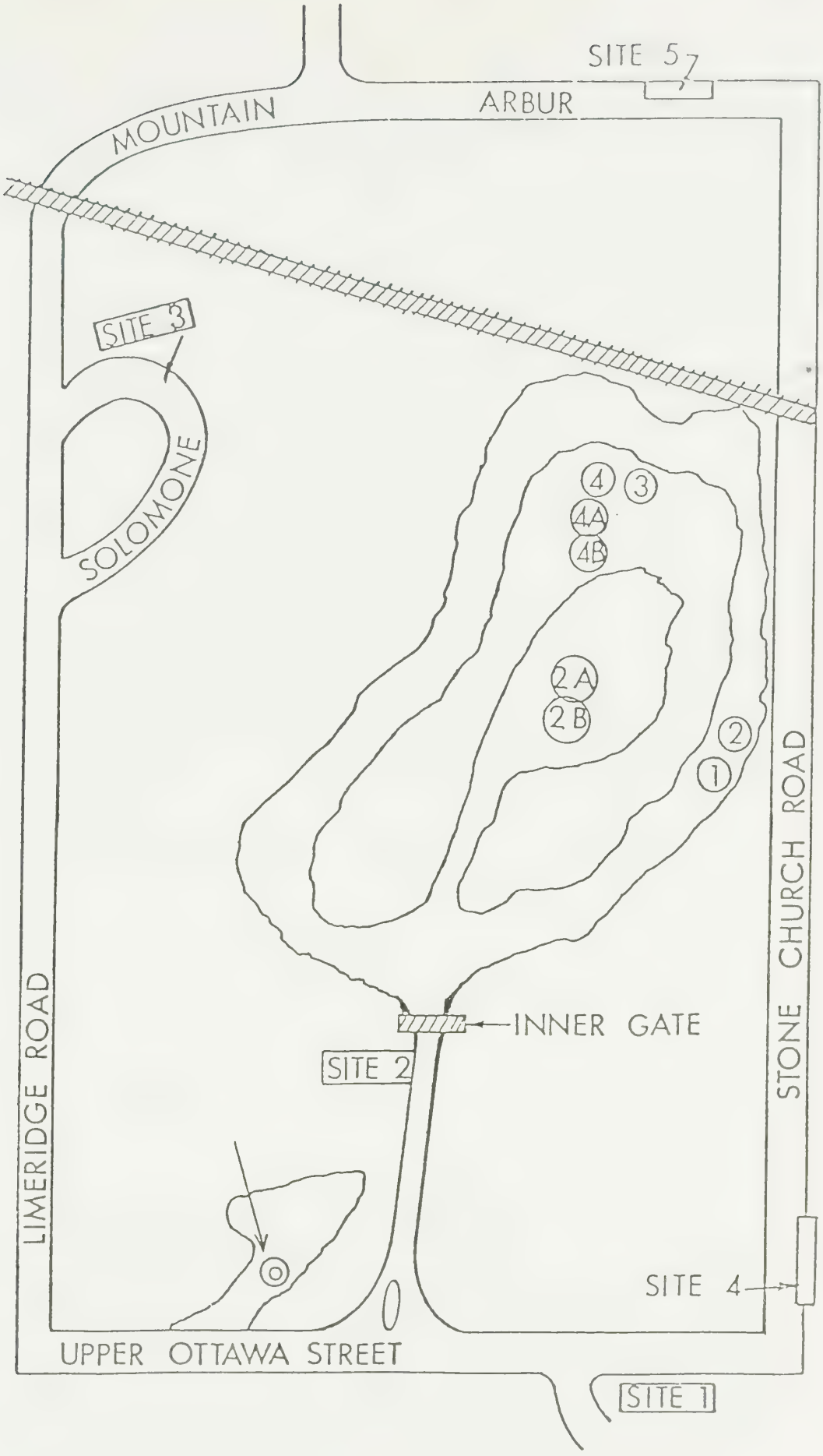


FIGURE 2.1-1 Approximate locations of the sampling sites.

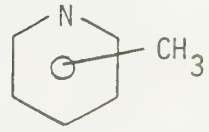
Thus a detected peak contains two pieces of information: the m/z leads to a MW and the intensity after appropriate calibration leads to a concentration of the chemical in ambient air.

d) The mass analyzer of the TAGA 3000 is a quadrupole capable of 1 atomic mass unit resolution, that is two chemicals that differ by 1 atomic mass unit will be distinguished from one another. However, two or more chemicals of the same nominal molecular weight will appear at the same m/z and will not be distinguished. This type of interference is generally alleviated by the use of a chromatographic technique, usually gas chromatograph (GC) coupled to a mass spectrometer (MS).

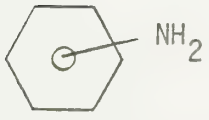
This technique has its own limitations that will not be discussed in this report since it was not used.

e) In order to achieve further separation of chemicals with the same molecular weight and at the same time retain the realtime monitoring capability of the TAGA 3000, a technique of chemical ionization (CI) mass spectrometry was developed for use with the TAGA 3000. This technique is based on the known thermochemical properties of chemicals. Figure 2.1-2 shows the complete scheme of chemical ionization reagents used to 'selectively' monitor chemical classes of volatile pollutants.

f) Even with this technique (CI/MS) some chemicals will still overlap and will not be distinguished. For example, the following two chemicals:



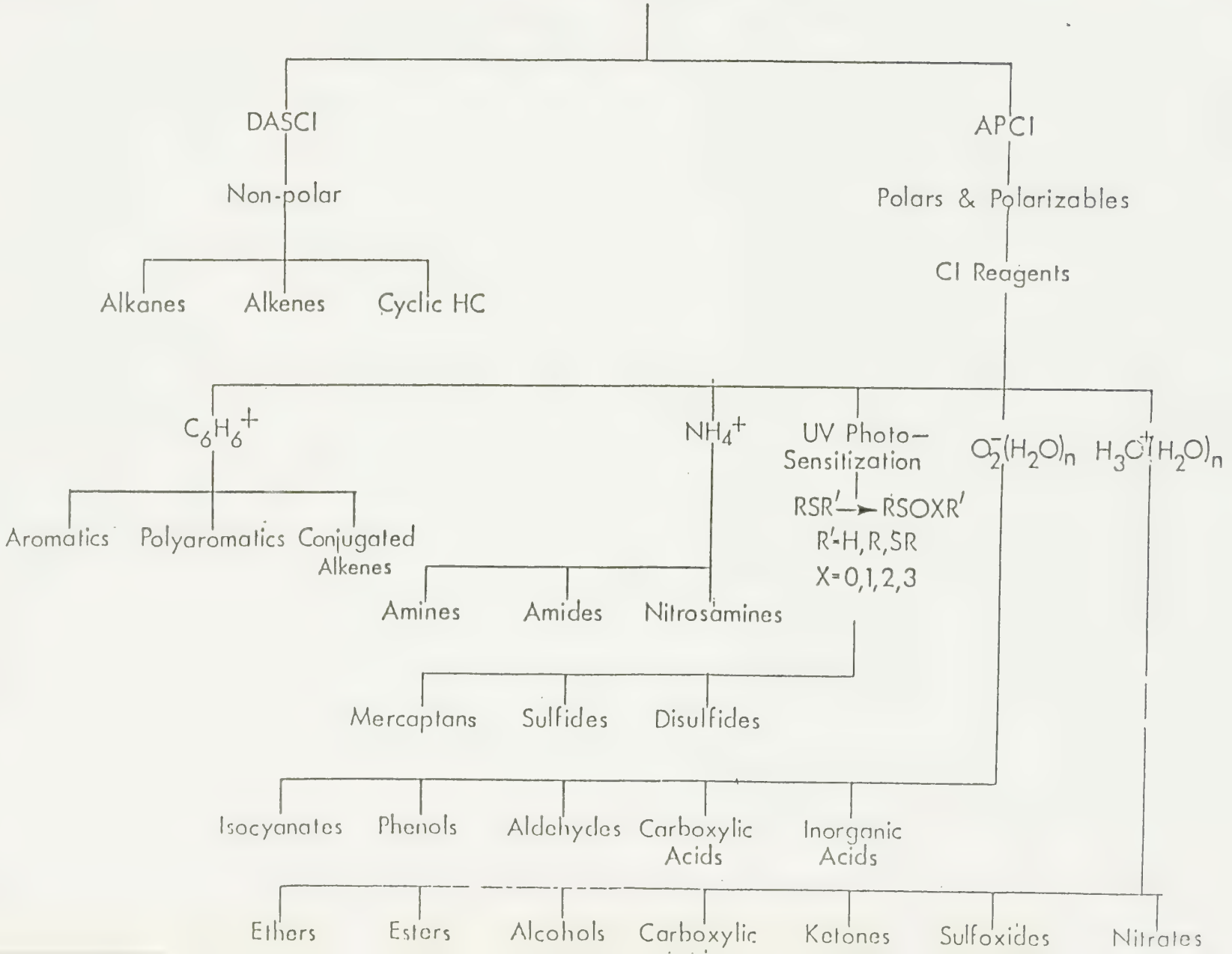
methylpyridine (picolines) MW = 93
m/z = 94



aniline MW = 93
m/z = 94

In the 1981 data (Appendix 2) when faced with this limitation, we made an assumption that the chemical associated with industrial use will be assigned for the detected m/z. Appendix 3 shows the detected peaks and the possible industrial chemicals that might lead to it. At the time this seemed a reasonable assumption based on the fact that the UOSL was used for industrial chemical disposal. However, due to biodegradation and chemical reactions among the disposed industrial wastes, some "new" chemicals can be formed.

FIGURE 2.1-2: SELECTIVE MONITORING OF VOLATILE POLLUTANTS



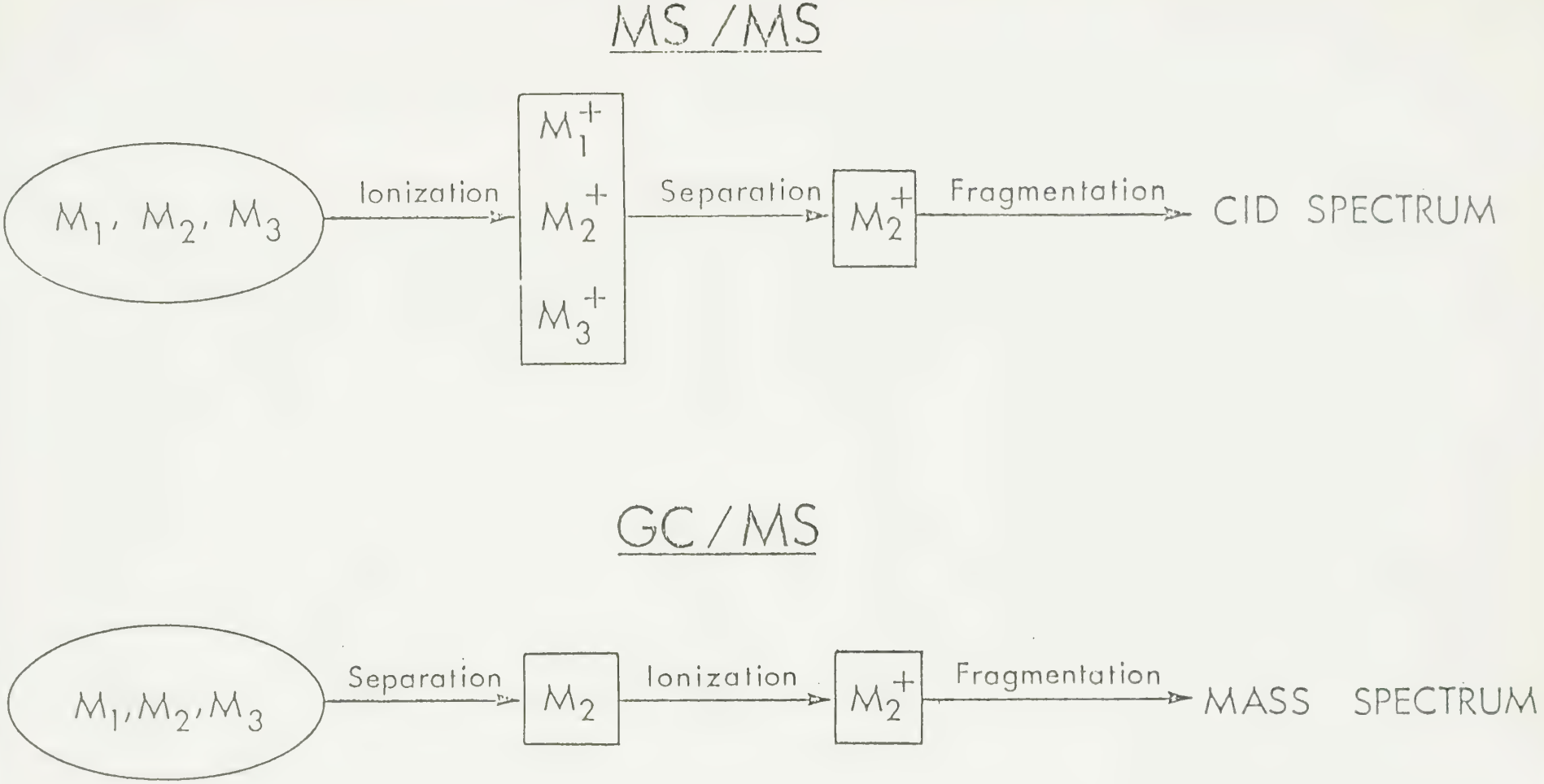
g) After the completion of our 1982 survey, a more sophisticated technique based on sequential mass spectrometry (MS/MS) became available. This technique, in one of its several operating modes, can be used as a separation/detection technique. The first mass spectrometer can be used for separating components of a mixture according to their m/z, a collision induced dissociation of the selected peaks leads to a mass spectral pattern that can be analyzed on the second mass spectrometer.

Figure 2.1-3 shows schematically the GC/MS and the MS/MS separation and detection.

Based on the potential of MS/MS for direct mixture analyses and component identification, it was agreed that this technique should be used to confirm or reject the identities of a select number of peaks detected in the 1981 survey (Appendix 2).

Since the TAGA 6000 MS/MS is not available yet in a mobile platform, it was decided that discrete air bag samples will be collected and brought back to SCIEX in Thornhill for MS/MS analysis.

FIGURE 2.1-3: SCHEMATIC REPRESENTATION OF THE SIMILARITIES BETWEEN GC/MS AND MS/MS ANALYTICAL TECHNIQUES



2.2 WORK PROGRAM

FDC Consultants Inc. was retained by the Study Group to perform a toxicity assessment of the tentatively identified chemicals in Appendix 2. The following list of priority chemicals was chosen by FDC for further study.

Proven Carcinogens (First Priority)

benzidine
dimethyl nitrosamine
ethylenimine
8-hydroxy quinoline
1-, 2- naphthylamine
xylenol
phenol

Reproductive Toxins (Second Priority)

acetaminophen
butyl acrylate
acrylic acid
thiocyanic acid

Indefinite Carcinogens (Third Priority)

acrolein
aniline
cresols
diphenylamine
hydroquinone
maleic anhydride
maleic hydrazide
quinone
sorbic acid
styrene
urethane

Potential Nitrosation Substrates (Fourth Priority)

dimethylamine
cyclohexylamine
carbofuran
bufencarb
carbaryl
nitrosodiphenylamine
nitrosophenol
tributylamine
triethanolamine

Upon mutual agreement between SCIEX and the Study Group, the following work program was initiated:

a) Discrete Tedlar bags of vented gases to be collected and analyzed on the MS/MS for the priority chemicals.

b) Calibration methodology development for the priority chemicals and generation of calibration constants for concentration estimates.

c) Concentration estimates of the priority chemicals in the 1981 survey.

d) Comparative field sampling and analysis in the priority chemicals using the TAGA 3000 Mobile for Ancaster Landfill, Upper Ottawa Street Landfill, Upper Ottawa residential area and Hamilton control area.

e) Field sampling and analysis for chlorinated hydrocarbons, using the TAGA 3000 mobile adapted for chlorinated hydrocarbons.

3.0 DISCRETE SAMPLE ANALYSIS BY MS/MS

3.1 GENERAL

Tedlar Air Bag Samples were collected on August 23, 1982 from Vent 1 of the Ancaster Landfill and Vents 1 and 4 of Upper Ottawa Street Landfill. The air bag samples were transported to SCIEX and analyzed on August 24, 1982 along with a blank air bag in order to eliminate any contribution from the bag.

Two more air bag samples were collected from a newly bored vent (approximately 8 feet below the surface) at the Upper Ottawa Street vent on January 11, 1983. The samples were immediately transported to SCIEX and analyzed within two hours of collection to minimize sample adsorption/degradation.

3.2 SAMPLE ANALYSIS

The sample analysis consisted of:

a) Single MS scans in both the positive and negative ion modes for each bag.

b) The peaks corresponding to the priority chemicals were selectively separated by the first MS and a collision induced (CID) mass spectrum was taken of the ion. Thus the procedure can simply be described as taking the mass spectrum of an ion in a mass spectrum.

c) The CID spectrum of the priority chemical standards was obtained under the same operating conditions of the instrument.

d) The spectra of the standards and the sample were then compared in order to confirm or reject the tentative assignments based on the single MS identification reported in the 1981 survey.

e) For peaks that did not match the priority chemical, the identity of the peak was assigned on the basis of its characteristic fragments. In this part the EPA/NIH Mass Spectral library was searched for comparative purposes.

3.3 RESULTS

The cumulative results for the priority chemicals in the five air bag samples can be classified according to the qualitative criteria: confirmed, unconfirmed, inconclusive evidence.

	Confirmed	Unconfirmed	Inconclusive
a) Proven Carcinogens			
benzidine		X	
dimethylnitrosamine		X	
ethylenimine		X	
8-hydroxy quinoline		X	
1-, 2-naphthylamine		X	
xylenol	X		
phenol	X		
b) Reproductive Toxins			
acetaminophen		X	
butylacrylate		X	
acrylic acid	X		
thiocyanic acid		X	
c) Indefinite Carcinogens			
acrolein		X	
aniline		X	
cresols	X		
diphenylamine		X	
hydroquinone		X	
maleic anhydride		X	
maleic hydrazide		X	
quinone		X	
sorbic acid		X	
styrene		X	
urethane		X	
d) Potential Nitrosation Products			
dimethylamine		X	
cyclohexylamine		X	
carbofuran		X	
bufencarb			X
carbaryl		X	
nitrosodiphenylamine		X	
nitrosophenol		X	
tributylamine		X	
triethanolamine		X	

In summary, the following priority chemicals have been conclusively identified:

acrylic acid

phenol

cresol

xylenol

The inconclusive evidence for carbaryl is due to the absence of the m/z 202 in the air bags collected on January 11, 1983. However, the air bags collected on August 23, 1982 showed the following ion intensities in counts per second (CPS):

Air Bag	∓CPS	Concentration
UOSL Vent 1	7000	0.94 ppb
UOSL Vent 4	-	0 ppb
Ancaster Vent 1	500	0.07 ppb

The concentration is based on the calibration of carbaryl (sensitivity 7448 cps/ppb). Since the threshold limit value (TLV) for carbaryl is 5000 ppb, the detected concentration in the vent is well below the permissible exposure level. The concentration of this chemical in the residential areas, as will be shown later, will be much less than the value in the vent due to dilution with ambient air.

For the unconfirmed peaks, alternate chemical identities were assigned based on fundamental fragmentation of patterns of chemical compounds. The alternate chemicals were discussed with the Study Group and submitted in a draft report. Only one alternate chemical poses potential toxic effects, methylpyridine. This compound is the alternate assignment to aniline. Subsequent to the initial identification, we have obtained a pure standard of methylpyridine and confirmed the identity of the m/z 94 as methylpyridine. Figure 3.3-1 shows the CID spectrum of m/z 94 in the air bag as well as o-, m-, and p- methylpyridine.

In order to compare the relative magnitudes of the confirmed toxic chemicals between an industrial landfill and municipal landfill, the air bag sample results are:

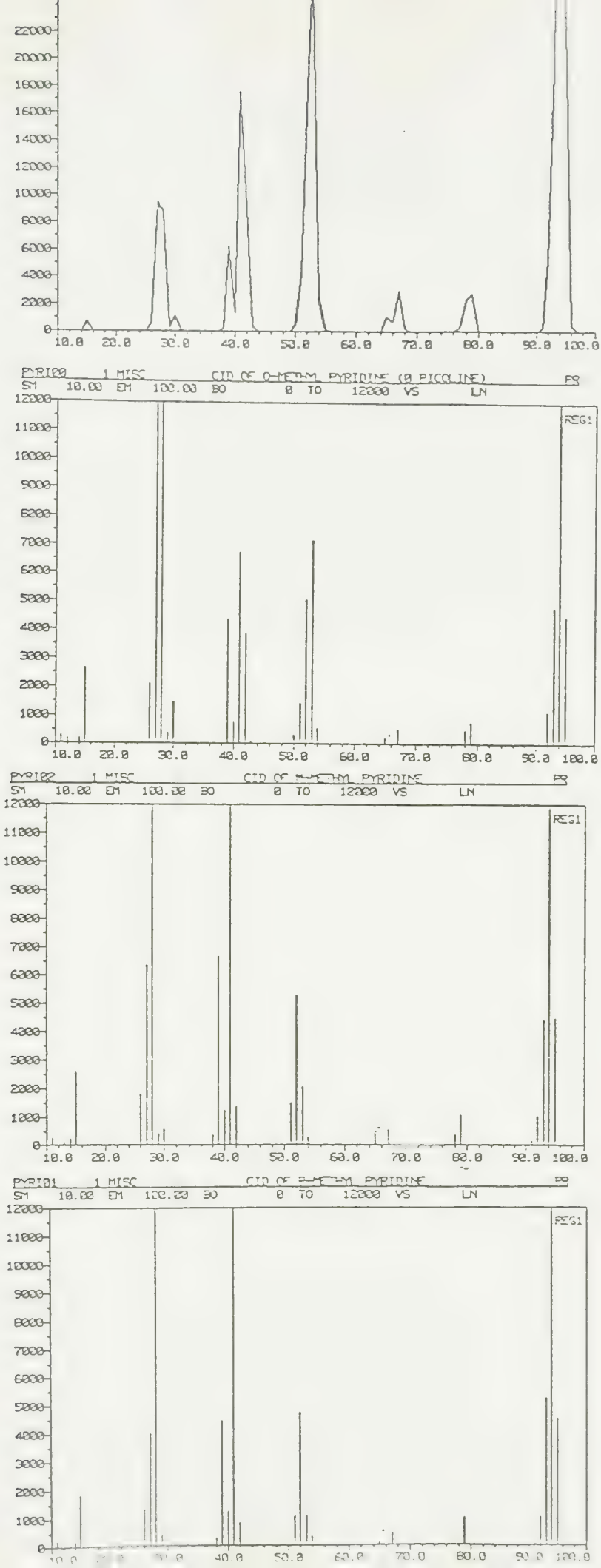

PYRI00 1 MISC CID OF O-METHYL PYRIDINE (O PICOLINE) PS
SM 10.00 EM 100.00 BO 0 TO 12000 VS LN
REG1
PYRI02 1 MISC CID OF M-METHYL PYRIDINE PS
SM 10.00 EM 100.00 BO 0 TO 12000 VS LN
REG1
PYRI01 1 MISC CID OF P-METHYL PYRIDINE PS
SM 10.00 EM 100.00 BO 0 TO 12000 VS LN
REG1

FIGURE 3.3-1

CID SPECTRA OF M/Z 94 IN AIR BAG AND o-, m-, AND p-METHYLPYRIDINE

Chemical	Upper Ottawa Vent 1 (%)	Vent 4 (%)	Ancaster Vent 1 (%)
methylpyridine	1604	6	100
acrylic acid	284	79	100
phenol	323	102	100
cresol	381	110	100
xylenol	718	135	100

These results show that vent 1 on UOSL has consistently higher concentrations than UOSL Vent 4 and Ancaster Vent 1. These results are consistent with our observation during the 1981 survey that Vent 1 was "active". This activity was manifested by condensation at the cooler pipe surface exposed to ambient air and the fact that the pipe was "hot" to touch.

4.0 CONCENTRATION ESTIMATES OF PRIORITY CHEMICALS FOR 1981 SURVEY

The TAGA calibration methodology and calibration results for the list of priority chemicals are given in Appendix 4. The relevant calibration constants for the confirmed toxic chemicals and the concentration estimates for the 1981 survey are shown in Table 4.0-1.

It is evident that Site 4 (Stone Church & Upper Ottawa Street) has the highest concentration compared to the other four sites. During sampling in August of 1981, site 4 was directly downwind of the landfill.

Table 4.0-1 shows clearly that the confirmed chemicals downwind of the site exist at very low concentrations, the highest observed is 4.72 ppb for acrylic acid at Stone Church and Upper Ottawa Street.

TABLE 4.0-1

CONCENTRATION ESTIMATES FOR CONFIRMED CHEMICALS (1981 SURVEY)

Chemical	Calibration Constant	TLV	Concentration (ppb)				
			Site 1	Site 2	Site 3	Site 4	Site 5
methylpyridine	1.666×10^7 cps/ppm	5 ppm	0.0097	0.008	0.016	0.024	0.011
carbaryl	7.448×10^3 cps/ppb	5 ppm	0.002	0.001	0.018	0.015	0.014
acrylic acid	6.762×10^5 cps/ppm	no data	1.22	1.37	3.49	4.72	3.16
phenol	6.030×10^3 cps/ppb	5 ppm	0.15	0.04	0.15	0.23	0.11
p-cresol	1.031×10^5 cps/ppb	5 ppm	0.001	0.001	0.005	0.007	0.004
2,4- xylenol	5.27×10^2 cps/ppb	no data	0.50	0.35	1.11	1.25	0.95

Legend

Site 1: Tekawitha School
Site 2: 10 metres from gate
Site 3: Lime Ridge Road
Site 4: Stone Church & Upper Ottawa Street
Site 5: Arbur Street

5.0 COMPARATIVE FIELD STUDIES

5.1 GENERAL

In order to assess any unique problems that might be associated with the industrial Upper Ottawa Street Landfill site and the associated residential area, comparative field surveys were conducted during May and June of 1982.

5.2 UPPER OTTAWA STREET LANDFILL/ANCASTER LANDFILL

The comparative study was conducted under the same conditions of instrument operation and field sampling. Two sites were monitored for each landfill, one upwind site and one downwind site. Table 5.2-1 shows the concentrations of confirmed chemicals and carbaryl.

The concentrations for the confirmed chemicals are all below 1 ppb. At such low concentrations no significant differences exist between any of the two sites.

5.3 RESIDENTIAL AREA COMPARISON

Comparative air quality surveys were conducted on eight locations in the Hamilton area. The peaks corresponding to the confirmed priority chemicals were quantified based on their respective calibration constants. Table 5.3-1 shows the results for all sites.

The results in Table 5.3-1 show that the concentrations estimated for Burlington and Stapleton and Hamilton Downtown are higher than the Upper Ottawa Street area. These two sites which are remote from the landfill are the only ones showing concentrations higher than 1 ppb. Based upon the results in Table 5.3-1, it is evident that the residential areas of Stone Church and King Ridge Plaza are not any different from the control residential areas on Chester, Mahony Park and Ottawa/Parkdale/Marton/Burlington. As expected the industrial areas (Burlington and Stapleton) and the urban area (Gage and King) show higher concentrations of the five chemicals. This has also been observed for the confirmed chemicals as well.

TABLE 5.2-1

UPPER OTTAWA/ANCASTER - SAMPLING DATE, JUNE 30, 1982

CHEMICAL	UPPER OTTAWA		ANCASTER	
	UPWIND NEAR LIME RIDGE RD. & UPPER KENILWORTH	DOWNWIND (NE) FROM STONE CHURCH	UPWIND NEAR HWY.2 AND SHAVERS ST.	DOWNWIND AT GATE SE-SW (23°C)
methylpyridine	0.22 ppb	0.12 ppb	0.07 ppb	0.09 ppb
carbaryl	0.00 ppb	0.07 ppb	0.00 ppb	0.05 ppb
acrylic acid	0.74 ppb	0.87 ppb	0.38 ppb	0.43 ppb
phenol	0.15 ppb	0.10 ppb	0.08 ppb	0.047 ppb
cresol	0.004 ppb	0.003 ppb	0.003 ppb	0.00 ppb
xylenol	0.40 ppb	0.34 ppb	0.26 ppb	0.25 ppb

TABLE 5.3-1

HAMILTON - SAMPLING DATE - JUNE 30, 1982

CHEMICAL	STONE CHURCH BY THE RESERVOIR	KING RIDGE PLAZA ON LIME RIDGE RD.	CHESTER AVENUE	BURLINGTON AND STAPLETON	MAHONY PARK	OTTAWA, PARKDALE, HARTON, BURLINGTON	HAMILTON DOWNTOWN AREA (GAGE & KING STS.)
methylpyridine	0.10 ppb	0.12 ppb	0.01 ppb	3.17 ppb	0.00 ppb	0.01 ppb	0.63 ppb
carbaryl	0.00 ppb	0.00 ppb	0.03 ppb	0.20 ppb	0.00 ppb	0.00 ppb	0.10 ppb
acrylic acid	0.80 ppb	0.42 ppb	0.68 ppb	3.6 ppb	0.00 ppb	0.00 ppb	2.22 ppb
phenol	0.067 ppb	0.05 ppb	0.22 ppb	1.29 ppb	0.00 ppb	0.33 ppb	1.28 ppb
cresol	0.003 ppb	0.002 ppb	0.003 ppb	0.017 ppb	0.00 ppb	0.00 ppb	0.29 ppb
xylenol	0.65 ppb	0.46 ppb	0.94 ppb	1.94 ppb	0.00 ppb	0.00 ppb	44.54 ppb

6.0 CHLORINATED HYDROCARBON SURVEY

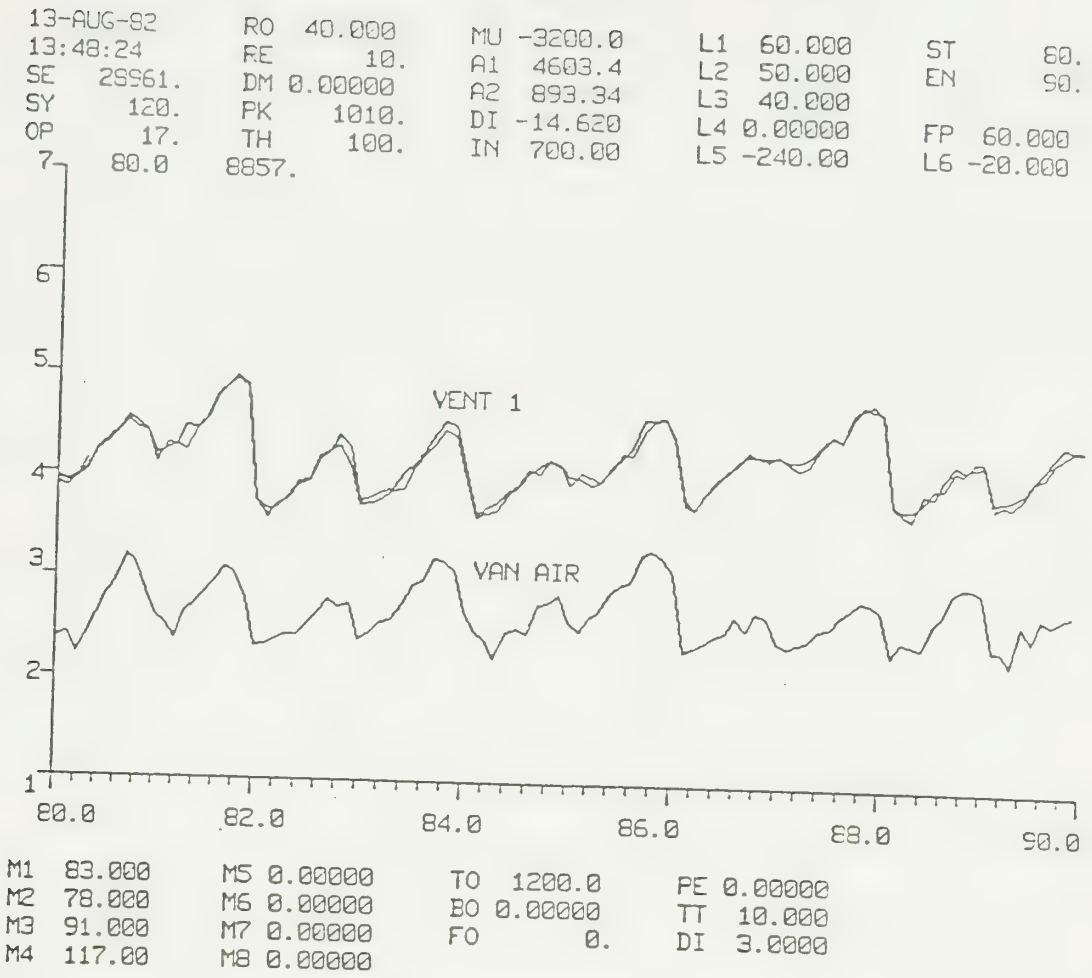
6.1 GENERAL

A special survey for chlorinated hydrocarbons was conducted on August 13, 1982 at Vents 1 and 4A of Upper Ottawa Street Landfill, and at the Blessed Kateri and Sterling schools. The SCIEX® mobile TAGA® 3000 was equipped with a specialized Direct Air Sampling Chemical Ionization (DASCI) source. The DASCI operates in the pressure range of 0.1 to 10 torr compared to the regular ion source which operates at 760 torr. The DASCI source was specially designed for the monitoring of chlorinated hydrocarbons. A discrete air bag sample was also collected from both Vents 1 and 4A. The sample was analyzed back at SCIEX® for total chlorine content.

6.2 RESULTS

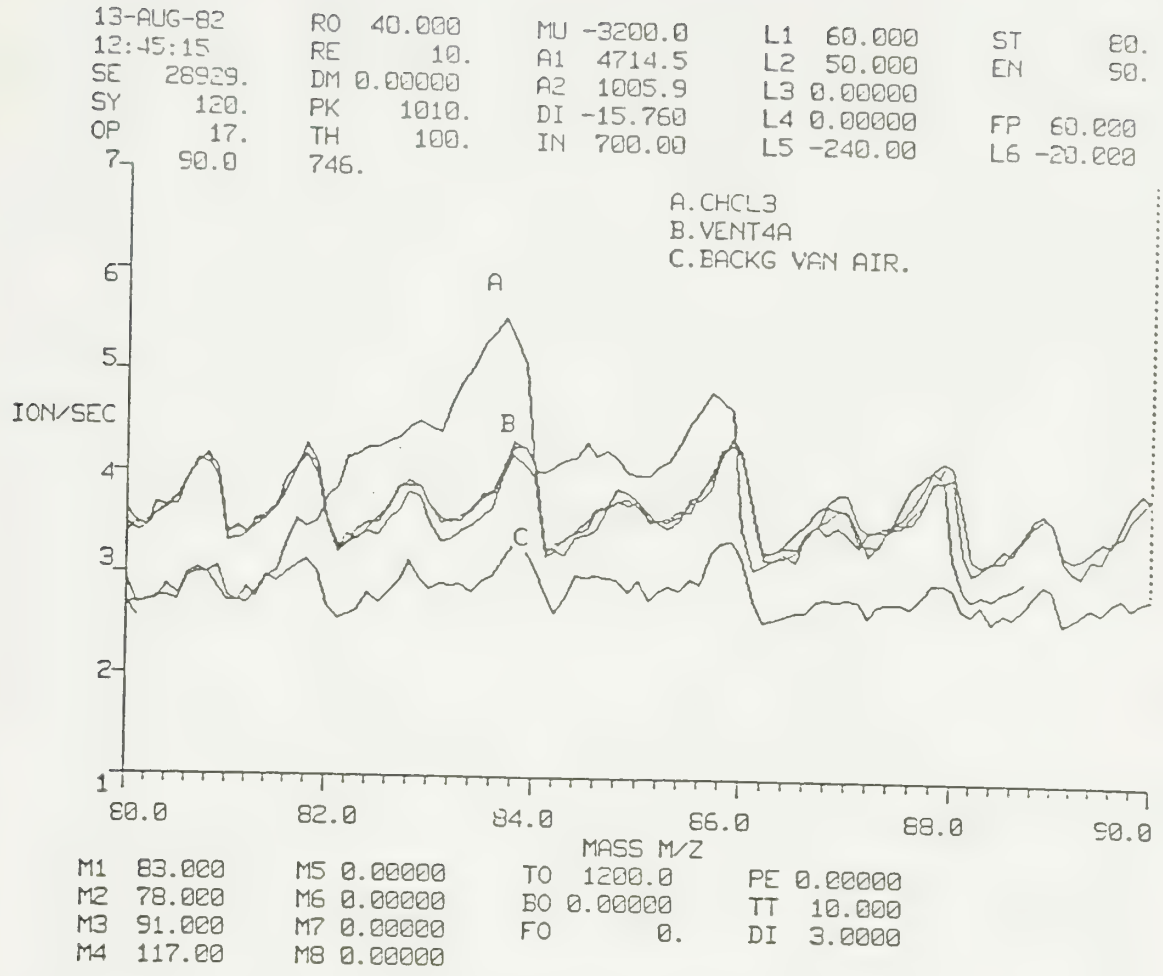
Figure 6.2-1 shows a realtime spectrum of Vent 1 and van air between m/z 80 and 90. This is the range suitable for detection of chloroform and breakdown products of higher chlorinated hydrocarbons. The peaks at 83 and 85 do not have the appropriate ratio for the chlorine isotopes. Figure 6.2-2 shows a similar experiment with Vent 4A. The same result was obtained: no chlorinated hydrocarbons at concentrations of greater than 1 ppb. Figure 6.2-2 shows the appropriate peaks when spiked with chloroform thus demonstrating the capability of detection.

The air bag analysis for total chlorides using the TAGA® MS/MS also indicated the absence of chlorinated hydrocarbons. Figure 6.2-3 shows the mass spectrum between m/z 15 and 250. The Cl^- peaks should have appeared at m/z 35 and 37. The absence of the peaks indicate that no chlorinated hydrocarbons exist in the bag at concentrations above 1 ppb. The latter is the detection limit for a number of chlorinated hydrocarbons using the TAGA® system.



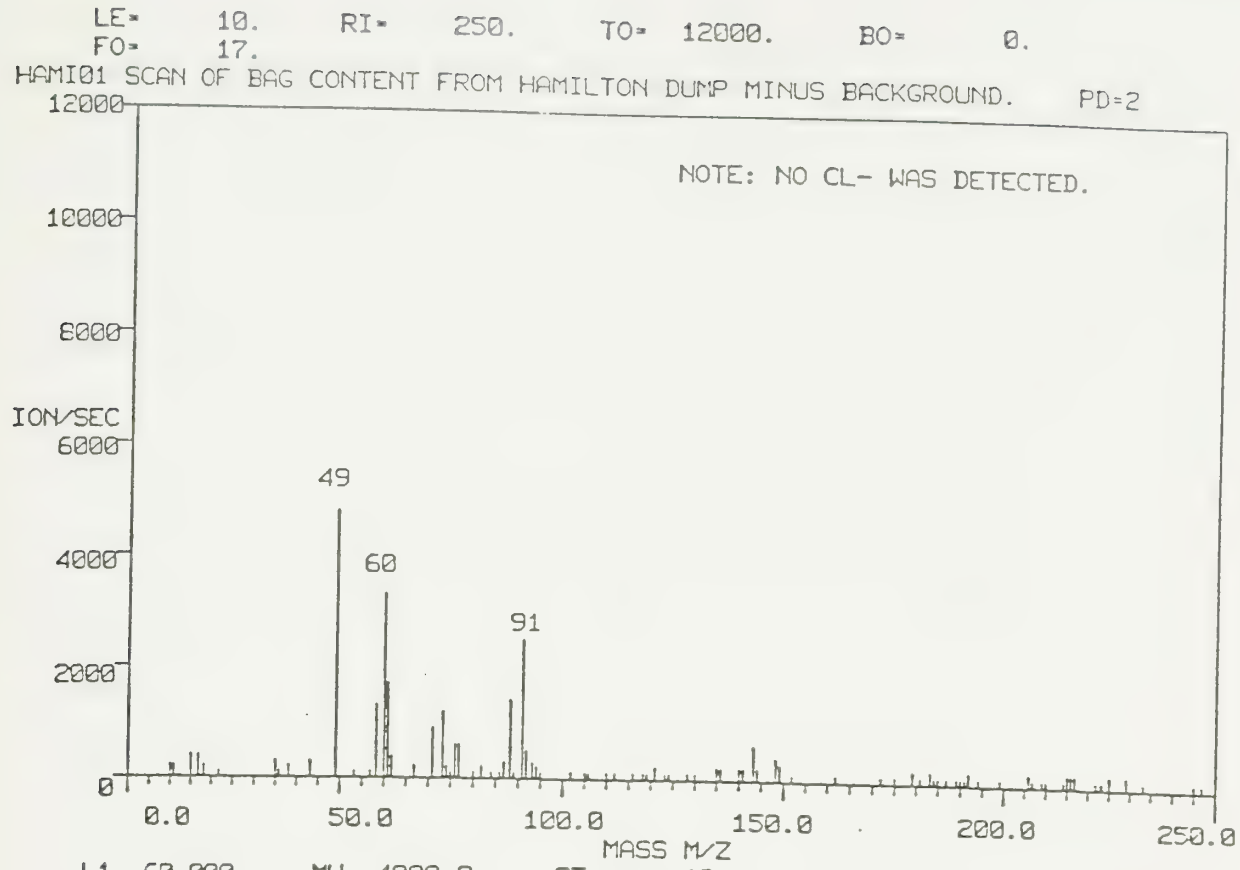
BACKGROUND VAN AIR USING DASCI AFTER VENT1.HI RE/RO

FIGURE 6.2-1



SITE#7 SAMPLING VENT#4A USING DASCI SOURCE, HI RE AND RO.

FIGURE 6.2-2



L1 -60.000	MU 4000.0	ST 10.	M1 19.300	F1 15.000
L2 -55.000	IN -650.00	EN 250.	M2 0.00000	F2 0.00000
L3 -45.000	FP -80.000	MM 0.00000	M3 0.00000	F3 0.00000
L4 -30.000			M4 0.00000	F4 0.00000
L5 250.00	TH 200.	PE 0.00000	M5 0.00000	F5 0.00000
L6 -25.000	PK 54.		M6 0.00000	F6 0.00000
	OP 0.		M7 0.00000	F7 0.00000
	SY 0.		M8 0.00000	F8 0.00000
RE 125.	DM 0.00000	R3 -35.000	Q2 3.5000	MO 0.00000
1R 0.	1D 0.00000	R1 -35.000	R2 -30.000	
C1 1.0000	C2 1.0000	C3 1.0000	C4 1.0000	QU 0.00000
C5 1.0000	C6 1.0000	C7 1.0000	C8 1.0000	
16-AUG-82	A1 5616.7	DI -1.9000	CG 4.5850	
10:44:00	A2 1276.0			

FIGURE 6.2-3

APPENDIX 1

ANALYSIS METHODOLOGY USING THE TAGA SYSTEM

1.1 Introduction

In order to fully comprehend the results and their significance, a brief summary of the TAGA™ methodology is necessary.

1.2 TAGA™ Technology

The TAGA™ technique is based on the use of mass spectrometry to identify and/or quantify trace species in gases at atmospheric or near atmospheric pressure. To make this approach practical for trace concentrations in the range of 1 in 10^6 to 1 in 10^{14}, it is necessary to produce a massive degree of pre-separation or pre-selection of the trace gas molecules from normal air constituents before their introduction into the mass spectrometer. This is done in Atmospheric Pressure Chemical Ionization (APCI) by an extremely rapid preferential ionization of the trace gas molecules using as reagents the ions produced in a primary ionization process from air. The primary ions are derived from water and oxygen for the positive and the negative modes, respectively.

In the positive modes, the reactant ions are dominated by the series $H_3O^+ (H_2O)_m$ which in turn ionize traces by simple non-fragmenting soft-ionization processes, as:

$$H_3O^+(H_2O)_n \begin{cases} \xrightarrow{T} TH^+ & (1) \\ \xrightarrow{T} TH_3O^+ & (2) \end{cases}$$

In the negative mode, the ions $O_2^-(H_2O)_n$, CO_3^- tend to be the dominant species which lead to simple non-fragmenting ionization processes such as:

$$O_2^-(H_2O)_n \begin{cases} \xrightarrow{T} T^- & (3) \\ \xrightarrow{T} (T\text{-}H)^- & (4) \end{cases}$$

The symbol T, in all equations, represents a trace consistituent in ambient air, carrier reagent gas.

In the positive ion mode, species with the highest gas phase basicity (proton affinity) tend to be the most reactive, while in the

negative ion mode, species with the highest gas phase acidity or electron affinity are the most reactive. Thus the ease of detection of traces will depend upon their relative basicities, acidities, ionization potentials or electron affinities to these primary reactant ions.

The classes of molecules that show high reactivity can be generally classified as those being polar or polarizable. Molecules containing a heteroatom such as O,N,P,S, halogen, a metal etc., and those containing conjugated double bonds fall into this category. Saturated alkanes, unconjugated alkenes, and cyclic hydrocarbons do not show any appreciable reactivity and thus the TAGA™ is "blind" to these chemicals under atmospheric pressure chemical ionization (APCI). A new ionization source developed at SCIEX™ overcomes this shortcoming if operated at reduced pressure (approximately 1 torr). This however, was not used for any of the surveys conducted at UOSL.

1.3 TAGA™ Selectivity

As discussed in the previous section, the classes of compounds that can be detected by the TAGA™ are those containing heteroatoms. This constitutes the first degree of selectivity. A second degree of selectivity depends on the utilization of the fact that reactivities of different chemical classes depend on the relative magnitudes of the thermochemical properties (basicities, acidities, ionization potentials and electron affinities) for the reagent and the trace components. For example, if ammonia is added to the carrier gas in parts per million or greater concentrations, the proton hydrates, $H_3O^+(H_2O)n$, will rapidly pass a proton to the ammonia forming ammonia hydrates as well as ammonia clusters, reactions (6) and (7) respectively.

$$H_3O^+(H_2O)_n + NH_3 \longrightarrow NH_4^+(H_2O)_{n-m} + m+1(H_2O) \qquad (6)$$

$$NH_4^+(H_2O)_n + NH_3 \longrightarrow NH_4^+(NH_3)(H_2O)_{n-1} + H_2O \qquad (7)$$

Since the basicity (proton affinity) of ammonia is so much higher than that of water, the ammonium ion, NH_4^+, will protonate fewer types of trace compounds than would the hydronium ion, H_3O^+. This will effectively "clean" up the spectrum by removing peaks due to oxygenated organics which were protonated by water, and intensify the peaks due to nitrogen based compounds. Thus the use of ammonia is said to "highlight" the nitrogen-containing species as amines, amides, etc.

Table 3.3-1 shows a summary of the chemical ionization reagents used to highlight chemicals of environmental concern. These reagents were used at the UOSL and its vicinity.

1.4 Data Acquisition

The TAGA™ 3000 system can acquire real time data in two generalized modes:

(a) Targeted compound analysis where the nature of the chemical is known. Thus prior calibration of the TAGA™ is performed and the selected chemicals up to 8 at a time, are monitored as a function of time while stationary or mobile. This mode was not used at UOSL since no prior knowledge of the chemicals was available.

(b) Scanning mode for unknowns. In this mode, the TAGA™ 3000 is set at a unit mass resolution in the mass-to-charge range of 2 to 500 atomic mass units. This range encompasses most of the volatile chemicals to be expected in ambient air. Because of the variety of chemicals that can have the same nominal mass-to-charge ratio, within 1 amu, a unique and unequivocal identification of a detected peak cannot be guaranteed. However, the use of selective chemical ionization reagents, Table 3.3-1 and "context" as well as tables of thermochemical parameters (proton affinities, ionization potentials, gas phase acidities, and electronegativities) can narrow the number of possible compounds to within two or three chemicals. Further detailed experimentation can be designed, in most cases, to achieve better identification. This limitation was resolved by developing the TAGA™ 6000 MS/MS system.

1.5 Data Reduction

The acquired data at the UOSL site can be reduced in two general approaches:

(a) an internally consistent single site analysis where the data for each sampling site is analyzed without reference to an upwind or background site. In this case, the data acquired under normal water and oxygen ion chemistries are analyzed and then subtracted from data obtained using other chemical ionization reagents. The resultant information can then be used to obtain a list of chemicals detected on the site.

TABLE 1.3-1

Summary of Chemical Ionization Reagents Used to Highlight Chemicals of Environmental Concern

Reagent	Highlighted Classes
	POSITIVE MODE:
$H_3O(H_2O)^+n$	Oxygenated Organics: ketones, alcohols, esters, etc.
NH_4^+	Nitrogen-Containing species: amines, amides, etc.
$C_6H_6^+$	Aromatics, polyaromatic hydrocarbons
photolysis pre-reactor	Sulfur compounds, alkenes
	NEGATIVE MODE:
$O_2^-(H_2O)n$	Phenolic group, carboxylic acids, aldehydes, SO_2, NO_2
photolysis pre-reactor	Sulfur compounds (RSH, RSR, RSSR)
Cl^-	Inorganic acids: H_2SO_4

(b) comparative data analysis where two sites are compared regarding their differences and similarities. This allows for background subtraction or correction. For example, two vents can be directly compared by the computer to determine whether there are qualitative or quantitative differences in their contents.

As a first approach, it is usually recommended that data be analyzed according to the internally consistent method, part (a) above. Depending on the results further analysis according to part (b) can then be efficiently and economically utilized. This approach has been adopted in this report.

1.6 Data Interpretation

The peak assignment, or identification is based on several factors as follows:

(a) Thermochemical parameters: proton affinity, ionization potential, gas phase acidity and electronegativity.

(b) Reactivity under various chemical ionization reagents and at APCI conditions.

(c) Context. The Merck Index and the EPA/NIH Mass Spectral data bases were consulted. Each detected peak was matched with all possible chemicals according to the above data base. A process of elimination based on the known behaviour in the TAGA™, (a) and (b) above, was used to arrive at a list of most likely chemicals. This list was further reduced by consulting the Merck Index regarding the uses of each chemical on the short list. Chemicals that were not used in large industrial quantities were eliminated as unlikely to be found in an industrial landfill site. It is to be noted that this is only an assumption to reduce the list of detected chemicals into a more manageable size. It is to be expected that some non-industrial use chemicals will be formed upon interaction of two industrial chemicals landfilled in the same location. As mentioned in Section 2.4, evidence of such interaction was observed in vent #1 during the sampling program.

A P P E N D I X 2

CHEMICALS TENTATIVELY IDENTIFIED

USING THE MOBILE TAGA 3000 SINGLE MS SYSTEM

2.1 Introduction

Extensive analysis of data for each site was performed as outlined in the previous section. This was followed by grouping the data into two generalized categories: chemicals that are normal constituents of ambient air and those considered unusual. The former group will not be included in this report. The unusual group of chemicals will be presented below.

2.2 Chemicals Detected in the Negative Ion Mode

The final results for this group of chemicals with all relevant information are included in Tables 2.2-1 and 2.2-2. The tables are divided into the following columns; mass-to-charge, M/Z; empirical formulae assignment; comments or identification whenever possible of the responsible chemical; and the sampling locations used in this survey. Table 2.2-1 shows the vents where a given chemical was detected, while Table 2.2-2 shows the same information for the residential sites. In other words, the two tables are identical except for the sampling locations. Table 2.2-1 deals with the vents while Table 2.2-2 shows the residential sites. The two tables can be used to determine whether a detected chemical originates in the UOSL site or is a constituent of the Hamilton urban environment. Chemicals detected on (Stone Church Road and Upper Ottawa Street) but not on Lime Ridge Rd or Arbur St. can most likely be attributed to the UOSL site, and similarly for chemicals detected at Tekokwitha School. It is to be noted that chemicals detected on the UOSL but not in the residential areas are not necessarily absent from the latter; these chemicals may exist at concentrations below the detection limits of the TAGA™ 3000 in realtime.

2.3 Chemicals Detected in the Positive Ion Mode

Similar to the results in Section 2.2, the final list of unusual chemicals detected in the positive ion mode is given in Table 2.3-1 for the vents and in Table 2.3-2 for the residential sites. The self explanatory tables are structured similar to Tables 2.2-1 and 2.2-2 and can be used for the same purposes.

TABLE 2.2-1

SUMMARY RESULTS OF CHEMICALS TENTATIVELY IDENTIFIED WITHIN THE VENTS USING THE NEGATIVE ION MASS SPECTRAL ANALYSES.

M/Z	ASSIGNMENTS	COMMENTS	VENT* 0	VENT 1	VENT 2	VENT 2A	VENT 2B	VENT 3	VENT 4	VENT 4A	
35	$^{35}Cl^-$	possibly from chlorinated organic compounds	ND	x	x	x	x	x	x	x	x
37	$^{37}Cl^-$	possibly from chlorinated organic compounds	ND	x	x	x	x	x	x	x	x
42	CNO^-	isocyanyl anion	ND				x				
45	$HCOO^-$	formic acid	ND	x		x	x			x	x
55	$C_3H_3O^-$	acrolein	ND		x						
57	CNS^-	thiocyanic acid	ND		x						
59	$C_2H_3O_2^-$	acetic acid	ND	x							x
61	$C_2H_5S^-$	ethyl mercaptan	ND			x					x
69	$C_3H_2O_2^-$	propiolic acid	ND	x	x						
71	$C_3H_3O_2^-$	acrylic acid/Oxid. Prod. of mass 55	ND	x	x					x	
72	$C_2H_2NS^-$	methyl thiocyanate	ND								
73	$C_3H_5O^-$	propanoic acid	ND	x		x	x			x	
75	$C_2H_3OS^-/C_2H_3O_3^-$	thio acetic acid/glycolic acid	ND		x						
77	$C_2H_5SO^-$	ethyl sulfonic acid	ND	x	x	x	x			x	
83	ClO_3^- (Cl=35)	chloric acid	ND		x						
85	ClO_3^- (Cl=37)/$C_4H_5O_2^-$	chloric acid/crotonic acid or methacrylic acid	ND		x		x			x	x
87	$C_3H_3O_3^-$	pyruvic acid	ND	x	x	x	x	x		x	x
89	$C_3H_6O_3^-$	lactic acid	ND		x			x			
91	$C_3H_7SO^-$	propyl mercaptan	ND			x	x				
92	$(C_2H_5NO_3)^-$	ethyl nitrate anion	ND							x	
93	$C_2H_5SO_2^-$	ethyl mercaptan	ND	x	x	x	x				
93	$C_6H_5O^-$	phenol	ND						x		
95	$CH_3O_3S^-$	methanesulfonic acid	ND								x
99	$C_5H_7O_2^-$	carboxylic acid	ND	x	x		x				x
101	$C_5H_9O_2^-$	valeric acid or isovaleric acid	ND	x	x	x	x			x	x
105	$C_4H_9SO^-$	butyl mercaptan	ND			x	x			x	x
107	$C_3H_7SO_2^-$	propyl mercaptan	ND	x							
107	$C_7H_8O^-$	cresol	ND		x				x		x
108	$C_6H_6NO^-$	nicotinyl alcohol	ND			x	x		x	x	x
109	$C_2H_5SO_3^-$	ethyl mercaptans	ND		x	x	x				x
111	$C_6H_7O_2^-$	sorbic acid	ND		x	x	x			x	x
115	$C_5H_7O_3^-/C_4H_3O_4^-/C_6H_{11}O_2^-$	levulinic acid/fumaric acid or maleic acid/n-caproic acid	ND	x	x	x	x	x	x		x
121	$C_4H_9SO_2^-$	butylmercaptan or ethyl sulfide	ND	x						x	x
121	$C_8H_9O^-/C_7H_5O_2^-$	benzoic acid/dimethylphenol	ND		x				x		
122	$C_6H_4NO_2^-$	nitrosophenol or picolinic acid	ND								x
123	$C_3H_7SO_3^-$	propyl mercaptan	ND				x			x	
125	$C_2H_5O_4S^-$	ethyl sulfate or dimethyl sulfate	ND				x			x	
127	$C_6H_4ClO^-/C_7H_{11}O_2^-$	chlorinated phenols/cyclohexane carboxylic acid	ND	x	x		x			x	x
129	$C_7H_{13}O_2^-$	heptanoic acid	ND	x	x						
131	$C_7H_{15}S^-$	hepta mercaptan	ND	x							
135	$C_8H_7O_2^-$	toluic acid or phenylacetic acid	ND		x						x
135	$C_5H_{11}SO_2^-$	pentyl mercaptan	ND								
137	$C_4H_9SO_3^-$	butyl mercaptan, ethyl sulfide	ND								x
139	$C_7H_4FO_2^-$(?)	fluorobenzoic acid(?)	ND		x					x	x
141	$C_6H_5O_4^-$(?)	kojic acid(?)	ND							x	x
142	$C_6H_8NOS^-$	MI	ND		x						x
143	$CH_3(CH_2)_6COO^-$	caprylic acid	ND	x	x	x		x	x		x
153	$C_7H_5O_2S^-$	thiosalicyclic acid	ND	x	x					x	x
157	$C_9H_{17}O_2^-$	pelargonic acid	ND	x				x	x		
167	$C_8H_7O_4^-$	dehydroacetic acid	ND								x
169	$C_7H_5OS_2^-$	dithiosalicylic acid	ND	x							x
171	$C_7H_7O_3S^-/C_{10}H_{19}O_2^-$	toluenesulfonic acid/capric acid	ND	x	x						x
183	$C_6H_3N_2O_3S^-$	diazobenzenesulfonic acid	ND	x							x
185	$C_2H_2IO_2^-$(?)	iodoacetic acid(?)	ND		x						

*Negative Mode Scan was not done for Vent 0 (ND = Not Determined)

TABLE 2.2-2

SUMMARY RESULTS OF CHEMICALS TENTATIVELY IDENTIFIED WITHIN THE RESIDENTIAL AREAS USING THE NEGATIVE ION MASS SPECTRAL ANALYSES.

M/Z	ASSIGNMENTS	COMMENTS	SITES 1	2	3	4	5
35	$^{35}Cl^-$	possibly from chlorinated organic compounds	x	x	x	x	x
37	$^{37}Cl^-$	possibly from chlorinated organic compounds	x	x	x	x	x
42	CNO^-	isocyanyl anion					
45	$HCOO^-$	formic acid	x	x			
55	$C_3H_3O^-$	acrolein					
57	CNS^-	thiocyanic acid				x	
59	$C_2H_3O_2^-$	acetic acid					
61	$C_2H_5S^-$	ethyl mercaptan					
69	$C_3H_2O_2^-$	propiolic acid					
71	$C_3H_3O_2^-$	acrylic acid/Oxid. Prod. of mass 55					x
72	$C_2H_2NS^-$	methyl thiocyanate				x	x
73	$C_3H_5O^-$	propanoic acid					x
75	$C_2H_3OS^-/C_2H_3O_3^-$	thio acetic acid/glycolic acid					
77	$C_2H_5SO^-$	ethyl sulfonic acid					
83	ClO_3^- (Cl=35)	chloric acid					x
85	ClO_3^- (Cl=37)/$C_4H_5O_2^-$	chloric acid/crotonic acid or methacrylic acid				x	x
87	$C_3H_3O_3^-$	pyruvic acid	x			x	x
89	$C_3H_6O_3^-$	lactic acid	x	x	x	x	x
91	$C_3H_7SO^-$	propyl mercaptan					
92	$(C_2H_5NO_3)^-$	ethyl nitrate anion					
93	$C_2H_5SO_2^-$	ethyl mercaptan					
93	$C_6H_5O^-$	phenol					
95	$CH_3O_3S^-$	methanesulfonic acid					
99	$C_5H_7O_2^-$	carboxylic acid					
101	$C_5H_9O_2^-$	valeric acid or isovaleric acid				x	x
105	$C_4H_9SO^-$	butyl mercaptan					
107	$C_3H_7SO_2^-$	propyl mercaptan					
107	$C_7H_8O^-$	cresol					
108	$C_6H_6NO^-$	nicotinyl alcohol					
109	$C_2H_5SO_3^-$	ethyl mercaptans					
111	$C_6H_7O_2^-$	sorbic acid					
115	$C_5H_7O_3^-/C_4H_3O_4^-/C_6H_{11}O_2^-$	levulinic acid/fumaric acid or maleic acid/n-caproic acid	x			x	x
121	$C_4H_9SO_2^-$	butylmercaptan or ethyl sulfide					
121	$C_8H_9O^-/C_7H_5O_2^-$	benzoic acid/dimethylphenol					
122	$C_6H_4NO_2^-$	nitrosophenol or picolinic acid					
123	$C_3H_7SO_3^-$	propyl mercaptan					
125	$C_2H_5O_4S^-$	ethyl sulfate or dimethyl sulfate					
127	$C_6H_4ClO^-/C_7H_{11}O_2^-$	chlorinated phenols/cyclohexane carboxylic acid				x	
129	$C_7H_{13}O_2^-$	heptanoic acid				x	
131	$C_7H_{15}S^-$	hepta mercaptan					
135	$C_8H_7O_2^-$	toluic acid or phenylacetic acid					
135	$C_5H_{11}SO_2^-$	pentyl mercaptan					
137	$C_4H_9SO_3^-$	butyl mercaptan, ethyl sulfide					
139	$C_7H_4FO_2^-$(?)	fluorobenzoic acid(?)					
141	$C_6H_5O_4^-$(?)	kojic acid(?)					
142	$C_6H_8NOS^-$	NI					
143	$CH_3(CH_2)_6COO^-$	caprylic acid				x	
153	$C_7H_5O_2S^-$	thiosalicyclic acid		x			
157	$C_9H_{17}O_2^-$	pelargonic acid					
167	$C_8H_7O_4^-$	dehydroacetic acid					
169	$C_7H_5OS_2^-$	dithiosalicylic acid					
171	$C_7H_7O_3S^-/C_{10}H_{19}O_2^-$	toluenesulfonic acid/capric acid					
183	$C_6H_3N_2O_3S^-$	diazobenzenesulfonic acid					
185	$C_2H_2IO_2^-$(?)	iodoacetic acid(?)					

LEGEND

Site 1= Tekawitha School
Site 2= 10 metres from gate
Site 3= Line Ridge Road
Site 4= StoneChurch Road and Upper Ottawa Street
Site 5= Arbur Street

TABLE 2.3-1

SUMMARY RESULTS OF CHEMICALS TENTATIVELY IDENTIFIED WITHIN THE VENTS USING THE POSITIVE ION MASS SPECTRAL ANALYSES

M/Z	ASSIGNMENTS	COMMENTS	VENTS								
			0	1	2	2A	2B	3	4	4A	4B
29	$C_2H_5^+$	fragment	x		x			x	x		
30	H_2CO^+	methane derivative		x		x					
31	CH_3O^+	fragment						x	x	x	
32	$(CH_3NH_2)H^+$	methylamine	x	x		x					
39	$C_3H_3^+$	fragment ion				x				x	x
43	$C_2H_3O^+$	fragment ion		x	x	x	x	x	x	x	
44	$C_2H_5NH^+$	ethylenimine		x		x					
45	$C_2H_5O^+$	fragment	x		x	x		x	x	x	
46	$[(CH_3)_2NH]H^+$	dimethylamine or ethylamine		x		x					
48	CH_5NO^+	methoxyamine		x	x	x					
49	CH_5S^+	methylmercaptan									
56	$C_3H_6N^+$	propionitrile		x		x					x
57	$C_3H_5O^+/C_4H_9^+$	acrolein or fragment		x	x		x			x	x
58	$(C_3H_7N)H^+$	allylamine								x	
59	$C_3H_6OH^+$	acetone or fragment ion	x		x			x	x		
60	$(C_3H_{10}N)^+$	acetamide and/or propanamine	x			x	x				x
61	$C_3H_9O^+/C_2H_5O_2^+/C_2H_9N_2^+$	ethyl methylether, propyl alcohol/ methyl formate/ethylenediamine	x								
63	$(C_2H_6O_2)H^+$	ethylene glycol				x				x	
65	$(CH_3SH.OH)^+$	methyl mercaptan derivative				x					
65	$C_5H_5^+$	fragment ion					x				
66	$C_5H_6^+$	fragment ion								x	
67	$C_5H_7^+$	cyclopentadiene			x						
69	$C_4H_5O^+/C_3H_5N_2^+$	fragment or furan/pyrazole	x	x	x		x	x	x	x	
70	$(C_4H_7N)H^+$	butane nitrile			x	x					
71	$(C_4H_6O)H^+$	crotonaldehyde, methyl vinyl ketone		x	x		x				
72	$C_3H_6NO^+$	acrylamide or hydracrylonitrile			x						
74	$(C_4H_{11}N)H^+/(C_3H_7NO)H^+$	butylamine/diethylamine/dimethylformamide		x		x	x				x
75	$[(CH_3)_2N_2O]H^+/[(C_2H_5)_2O]H^+$	dimethylnitrosoamine/diethylether or t-butanol									
76	$(C_3H_9NO)H^+$	possibly an amjno alcohol			x	x	x				
77	$C_3H_9O_2^+$	methyl cellosolve, or propylene glycol or trimethylene glycol			x						
79	$(C_2H_6OS)H^+$	dimethyl sulfoxide or 2-mercaptoethanol						x		x	
80	$(C_5H_5N)H^+$	pyridine		x	x	x	x		x	x	x
81	$C_4H_5N_2^+$	pyrazine/pyridazine/pyrimidine		x	x					x	
82	$C_6H_{10}^+$	cyclohexane or 2,3-dimethyl-1,3-butadiene								x	
83	$C_5H_7O^+/C_6H_{11}^+$	methylfuran or fragment or 2,3,dimethyl-1,3-butadiene	x	x	x	x	x	x	x	x	
85	$C_4H_5O_2^+/C_5H_9O^+$	diketene/cyclopentanone	x	x	x	x	x	x	x	x	x
87	$(C_4H_7O_2)^+/C_5H_{11}O^+$	methylacrylate or methacrylic acid/NI			x						
89	$(C_4H_8O_2)H^+/(C_5H_{12}O)H^+$	esters and/or alcohols		x			x				
90	$C_4H_{12}NO^+/C_3H_8NO_2^+$	2-amino-2-methyl-1-propanol/urethan			x	x					
93	$(C_3H_7SH.OH)^+$	propylmercaptan derivative			x						
93	$C_3H_9O_3^+$	glycerol		x			x				
94	$(C_6H_7N)H^+/C_6H_5NH_2)H^+$	methyl pyridine/aniline		x		x	x				x
95	$(C_2H_5SHO_2H)^+/[(CH_3)_2SO_2H]^+$	ethyl mercaptan and/or methyl sulfide derivatives		x	x	x					
95	$(C_5H_6N_2)H^+/(C_6H_6O)H^+$	aminopyridine/phenol					x	x	x		
96	$C_5H_6NO^+$	pyridine-1-oxide		x		x	x				
97	$C_5H_5O_2^+/C_6H_9O^+/CH_5O_3S^+$	furfural/1-pentol/methane sulfonic acid	x	x	x	x		x	x	x	
99	$C_6H_{11}O^+/C_5H_7O_2^+/C_4H_3O^+$	cyclohexanone/lactone/maleic anhydride		x	x	x	x		x	x	
100	$C_6H_{14}N^+$	cyclohexylamine					x				
101	$C_6H_{13}O^+/C_5H_9O_2^+/C_4H_5O_3^+$	hexanone/ethylacrylate/succinic anhydride	x		x		x	x	x		
102	$(C_6H_{15}N)H^+$	alkylamine				x					
103	$(C_6H_{14}O)H^+/(C_5H_{10}O_2)H^+$	diisopropyl ether/propyl acetate/pyruvic acid, methyl ester/methyl butyrate		x			x				x
104	$C_8H_8^+$	M^+ ion of styrene			x	x	x			x	
106	$C_4H_{12}NO_2^+$	2-amino-2-methyl-1,3-propanediol or diethanolamine	x								
107	$(C_7H_6O)H^+$	benzaldehyde			x		x		x	x	
108	$C_7H_7^+.NH_3/C_7H_{10}N^+$	tropylium-ammonia cluster/benzylamine or ethyl pyridine or methyl aniline	x	x	x	x	x			x	x
109	$C_6H_5O_2^+/C_7H_9O^+$	quinone/cresols		x	x						
110	$C_6H_8NO^+$	aminophenols	x		x	x	x			x	
111	$C_6H_7NO_2^+$	hydroquinone	x	x	x	x	x	x	x	x	x
111	$(C_2H_5SHO_3H)^+$, $[(CH_3)_2SO_3H]^+$	ethylmercaptan or dimethylsulfide				x					
113	$C_4H_5N_2O_2^+/C_6H_9O_2^+/$ $C_7H_{13}O^+/C_6H_{13}N_2^+$	maleic hydrazide/sorbic acid/ cycloheptanone/triethylenediamine			x		x			x	

TABLE 2.3-1 (continued)

M/Z	ASSIGNMENTS	COMMENTS	VENTS								
			0	1	2	2A	2B	3	4	4A	4B
115	$(C_7H_{14}O)H^+$	2-heptanone					x				
116	$(C_5H_9NS)H^+/C_9H_8^+$	isobutyl thiocyanate/indene				x	x			x	
117	$(C_7H_{16}O)H^+/(C_6H_{12}O_2)H^+$	heptanol and/or butylacetate			x		x		x		
118	$C_6H_{16}NO^+$	2-diethylaminoethanol		x	x		x				
119	$C_4H_7O_2S^+/C_8H_7O^+/$ $C_6H_{15}O_2^+$	3-sulfolene/benzofuran cellosolve (2-butoxyethanol)			x		x	x			
120	$C_5H_{14}NO_2^+$	2-amino-2-ethyl-1,3-propanediol				x	x				
121	$C_5H_{13}O_3^+/C_8H_9O^+$	methyl carbitol/acetophenone			x		x			x	x
122	$C_8H_{12}N^+$	N.I.		x							x
123	$C_8H_{11}O^+/C_7H_7O_2^+$	xylenol, phenethyl alcohol/benzoic acid	x	x	x				x		
124	$C_6H_6NO_2^+$	nitrosophenol	x	x		x	x			x	
125	$C_8H_{13}O^+$	N.I.				x					
126	$C_8H_{16}N^+(?)$	coniceine (?)	x							x	
127	$C_3H_7N_6^+$ or $C_6H_7O_3^+$	melamine or pyrogallol			x		x				
128	$C_5H_6NOS^+$	pyrithione	x		x	x	x			x	
129	$C_7H_{13}O_2^+/C_8H_{17}O_2^+$	n-butyl acrylate/ethyl amyl ketone or hexyl methyl ketone			x		x			x	
130	$C_6H_{12}NS^+$	isoamyl thiocyanate					x				
131	$C_7H_{15}O_2^+/C_8H_{19}O^+$	ester/alcohol or ether			x		x				
132	$C_9H_{10}N^+$	skatole					x				
133	$C_9H_9O^+/C_6H_{13}O_3^+$	cinnamaldehyde, 2,2,dimethyl-1, 3-dioxolane-4-methanol or 2,5-tetrahydrofurandimethanol	x		x						
134	N.I.	N.I.					x		x		
135	$C_6H_{15}SO^+$	hexylmercaptan or dipropyl sulfide derivatives					x			x	x
136	$C_7H_6NS^+$	benzothiazole		x		x	x				x
137	$C_8H_9O_2^+/C_9H_{13}O^+$	esters/alcohols, ethers									x
138	$C_8H_{12}NO^+$	phenylethanolamine			x	x	x				
139	$C_8H_{11}O_2^+/C_6H_7N_2O_2^+/$ $C_4H_{11}O_3S^+$	cresols/nitroanilines/ 2-(ethylsulfonyl) ethanol	x	x	x	x	x			x	x
140	$C_3H_{10}NO_3S/C_6H_6NO_3^+$	n-methyltaurine/nitrophenols			x	x	x				
141	$C_6H_{13}N_4^+$	methenamine (?)	x				x			x	x
142	$C_8H_{16}NO^+$ (?)	n-acetylcyclohexylamine (?)		x		x	x			x	
143	$C_8H_{15}O_2^+$	cyclohexane carboxylic acid, methyl ester		x	x		x	x			x
144	$C_{10}H_{10}N^+$	naphthylamine				x	x				x
145	$C_6H_9O_4^+/C_8H_{17}O_2^+/$ $C_{10}H_9O^+$	fumaric acid, dimethyl ester or lactide/ ester compound/naphthol					x			x	
146	$C_9H_8NO^+$	8-hydroxyquinoline			x	x	x				
147	N.I.	N.I.								x	
148	$C_8H_6NO_2^+$ (?)	pthalimide (?)					x				
149	$C_8H_5O_3^+$	pthalic anhydride			x			x	x		
150	$C_6H_{16}NO_3^+$	triethanolamine	x			x			x		x
151	$C_6H_{15}O_4^+$	triethylene glycol				x	x				
152	$C_8H_{10}NO_2^+$	acetaminophen				x	x				
153	$C_8H_9O_3^+$	cresotic acids		x	x	x	x				x
154	$C_7H_8NO_3^+$	amino salicylic acid		x			x			x	
155	$C_7H_7O_2S^+/C_4H_{13}FN_2OP^+/$ $C_{10}H_{19}O^+$	Thiosalicylic acid/Dimefox/-Terpineol/citronellal			x	x	x	x			
156	NI	NI				x	x				
157	$C_{10}H_{21}O^+$	citronellol, menthol or rhodinol					x		x		x
158	$C_{10}H_{24}N^+$	Diisoamylamine		x		x	x				x
159	$C_6H_7O_3S^+$	benzene sulfonic acid		x	x		x				
160	$C_6H_{10}NO_2S^+$	citiolone	x		x		x				x
161	NI	NI					x				
162	NI	NI	x				x				
163	$C_8H_{19}SO^+$	octyl mercaptan or dibutylsulfide derivatives			x	x	x				
164	$C_6H_{14}NO_4^+$	2-Nitro-2propyl-1,3- propanediol					x	x	x		
165	$C_8H_9N_2O_2^+/C_{10}H_{13}O_2^+/$ $C_{11}H_{17}O^+$	phthalamide/ethylphenyl acetate/ Jasmone					x				
166	$C_{10}H_{16}NO^+$	(aminopropyl) benzyl alcohol					x				
167	$C_9H_{11}O_3^+/C_9H_{15}N_2O^+$	ethyl salicylate or ethyl vanillin/ 5-amino-2-butoxypyridine					x			x	
168	$C_{12}H_{10}N^+$	carbazole					x				
169	$C_8H_9O_4^+$	dehydroacetic acid	x	x	x		x				x
170	$(C_{12}H_{11}N)H^+$	diphenylamine		x	x	x	x			x	x
171	$C_{12}H_{11}O^+$	phenylphenol			x	x	x			x	
172	$C_7H_{11}ClN_3^+/C_8H_{18}N_3O^+$	crimidine/2-heptanone, semicarbazone		x		x	x				
173	$C_6H_9N_2O_2S^+/C_{10}H_{21}O_2^+$	Porofor BSH/octyl acetate			x		x				x

TABLE 2.3-1 (continued)

M/Z	ASSIGNMENTS	COMMENTS	VENTS								
			0	1	2	2A	2B	3	4	4A	4B
174	$C_6H_8NO_3S^+$	sulfanilic acid		x	x		x				
175	$C_7H_{11}O_5^+$	adipic acid, dimethyl ester or dimethoxane					x				
176	$C_6H_7FNO_2S^+$	sulfanilyl fluoride		x			x			x	x
177	$C_9H_{21}SO^+$	nonylmercaptan derivative				x	x				
178	$C_{10}H_{12}NO_2^+$	acetoacetanilide				x	x				
179	$C_8H_{19}SO_2^+$	octylmercaptan or dibutyl sulfide derivative					x				
180	$C_{10}H_{14}NO_2^+$	IPC	x		x		x				
181	$C_{10}H_{13}O_3^+$	2-phenoxyethanol acetate			x	x	x				
182	$C_{12}H_{24}N^+$	dicyclohexylamine									x
183	$C_6H_{17}FN_2OP^+$ /$C_{11}H_{19}O_2^+$/ $C_6H_{15}O_6^+$	mipafox/geraniol, formate/sorbitol	x	x							x
184	$C_4H_{11}NO_3PS^+$	acephate									x
185	$C_{12}H_{13}N_2^+$	benzidine		x							x
186	$C_{12}H_{28}N^+$	tributylamine		x	x		x				x
188	NI	NI		x	x						
190	$C_{12}H_{16}NO^+$(?)	benzoylpiperidine, or ethyl crotonanilide(?)			x		x				
192	$C_{12}H_{18}NO^+/C_{13}H_{22}N^+$	N,N-diethyl-m-toluamide/2,6-Di-tert butylpyridine			x		x				
193	$C_{13}H_{21}O^+/C_{12}H_{17}O_2^+$	ionone/isoamyl benzoate				x	x			x	
194	$C_{11}H_{16}NO_2^+$	isobutyl-p-aminobenzoate		x	x		x		x		
196	$C_{11}H_{17}NS^+$	1-naptholisothiocyanate			x				x		
197	$C_{11}H_{14}ClO^+/C_{12}H_{20}O_2^+$	dowicide/geraniol, acetate or linalyl acetate	x								
198	$C_{13}H_{12}NO^+$	benzanilide	x								
199	$(C_{12}H_{10}N_2O)H^+$	N-nitrosodiphenylamine		x							x
201	$C_6H_5N_2O_6^+$	2,4-dinitroresorcinol		x							x
202	$C_{12}H_{12}NO_2^+$	carbaryl			x						
203	$C_{10}H_{19}O_4^+$	ethyl adipate/hexyleneglycol, diacetate		x			x				x
204	$C_9H_{18}NO_2S^+/C_{10}H_{22}NOS^+$	Lethane/pebulate		x	x		x			x	
206	NI	NI			x					x	
208	$C_{12}H_{18}NO_2^+$	promecarb		x							
214	$C_{13}H_{12}NO_2^+$	salicylanilide				x				x	
217	$C_{11}H_{21}O_4^+$	esters			x	x	x				
218	NI	NI					x				
219	$C_7H_7O_6S^+$	sulfosalicylic acid					x				
220	NI	NI		x			x				
221	$C_4H_8Cl_2O_4P^+/C_{11}H_9O_5^+$ /$C_{15}H_{25}O^+SO^+$	Dichlorvos/Purpurogallin/DBMC or santalol or butylated hydroxytoluene					x				
222	$C_{12}H_{16}NO_3^+/C_{13}H_{20}NO_2^+$	carbofuran/bufencarb					x			x	
223	$C_{10}H_{23}O_3S^+$	decylmercaptan or dipentyl sulfide derivatives				x					
225	$C_{10}H_9O_4S^+/C_7H_{18}O_6P^+$	cassella's acid or napthol sulfonic acid/mevinphos/		x							
226	$C_{13}H_{12}N_3O^+$	Tinuvin P,		x							
234	NI	NI								x	
235	$C_{13}H_{19}N_2O_2^+/C_{17}H_{15}O^+$ $C_8H_{16}N_2O_4P^+/C_{10}H_{17}N_2OS_2^+$	lenacil/dibenzalacetone/ 0,0,diethyl-0-(3-methyl-5-pyrazolyl)phosphate or Quinomethionate							x		
240	$C_{10}H_{10}NO_4S^+/C_{16}H_{17}NO^+$	amino-napthol-sulfonic acid/ diphenamid		x							
246	$C_{13}H_{16}N_3O_2^+$	pyrolan		x						x	
248	NI	NI		x						x	

TABLE 2.3-2

SUMMARY RESULTS OF CHEMICALS TENTATIVELY IDENTIFIED WITHIN THE RESIDENTIAL AREAS USING THE POSITIVE ION MASS SPECTRAL ANALYSES

M/Z	ASSIGNMENTS	COMMENTS	SITES 1	2	3	4	5
29	$C_2H_5^+$	fragment	x	x	x	x	x
30	H_2CO^+	methane derivative					x
31	CH_3O^+	fragment					x
32	$(CH_3NH_2)H^+$	methylamine			x		
39	$C_3H_3^+$	fragment ion			x		
43	$C_2H_3O^+$	fragment ion	x	x	x	x	x
44	$C_2H_5NH^+$	ethylenimine					
45	$C_2H_5O^+$	fragment	x	x	x		x
46	$[(CH_3)_2NH]H^+$	dimethylamine or ethylamine					
48	CH_5NO^+	methoxyamine					x
49	CH_5S^+	methylmercaptan					x
56	$C_3H_6N^+$	proponitrile					
57	$C_3H_5O^+/C_4H_9^+$	acrolein or fragment			x	x	x
58	$(C_3H_7N)H^+$	allylamine					
59	$C_3H_6OH^+$	acetone or fragment ion		x	x	x	x
60	$(C_3H_{10}N)^+$	acetamide and/or propanamine					
61	$C_3H_9O^+/C_2H_5O_2^+/C_2H_9N_2^+$	ethyl methylether, propyl alcohol/ methyl formate/ethylenediamine		x	x		x
63	$(C_2H_6O_2)H^+$	ethylene glycol					
65	$(CH_3SH.OH)^+$	methyl mercaptan derivative					
65	$C_5H_5^+$	fragment ion					
66	$C_5H_6^+$	fragment ion					
67	$C_5H_7^+$	cyclopentadiene			x		
69	$C_4H_5O^+/C_3H_5N_2^+$	fragment or furan/pyrazole	x		x	x	x
70	$(C_4H_7N)H^+$	butane nitrile		x			
71	$(C_4H_6O)H^+$	crotonaldehyde, methyl vinyl ketone			x		x
72	$C_3H_6NO^+$	acrylamide or hydracrylonitrile			x	x	
74	$(C_4H_{11}N)H^+/(C_3H_7NO)H^+$	butylamine/diethylamine/dimethylformamide					
75	$[(CH_3)_2N_2O]H^+/[(C_2H_5)_2O]H^+$	dimethylnitrosoamine/diethylether or t-butanol			x		
76	$(C_3H_9NO)H^+$	possibly an amino alcohol					
77	$C_3H_9O_2^+$	methyl cellosolve, or propylene glycol or trimethylene glycol			x	x	x
79	$(C_2H_6OS)H^+$	dimethyl sulfoxide or 2-mercaptoethanol			x		
80	$(C_5H_5N)H^+$	pyridine					
81	$C_4H_5N_2^+$	pyrazine/pyridazine/pyrimidine			x		x
82	$C_6H_{10}^+$	cyclohexane or 2,3-dimethyl-1,3-butadiene					
83	$C_5H_7O^+/C_6H_{11}^+$	methylfuran or fragment or 2,3,dimethyl-1,3-butadiene	x	x	x		x
85	$C_4H_5O_2^+/C_5H_9O^+$	diketene/cyclopentanone	x	x	x		
87	$(C_4H_7O_2)^+/C_5H_{11}O^+$	methylacrylate or methacrylic acid/NI		x	x		x
89	$(C_4H_8O_2)H^+/(C_5H_{12}O)H^+$	esters and/or alcohols					
90	$C_4H_{12}NO^+/C_3H_8NO_2^+$	2-amino-2-methyl-1-propanol/urethan				x	
93	$(C_3H_7SH.OH)^+$	propylmercaptan derivative					
93	$C_3H_9O_3^+$	glycerol					
94	$(C_6H_7N)H^+/(C_6H_5NH_2)H^+$	methyl pyridine/aniline					
95	$(C_2H_5SHO_2H)^+/[(CH_3)_2SO_2H]^+$	ethyl mercaptan and/or methyl sulfide derivatives					
95	$(C_5H_6N_2)H^+/(C_6H_6O)H^+$	aminopyridine/phenol	x	x		x	x
96	$C_5H_6NO^+$	pyridine-1-oxide					
97	$C_5H_5O_2^+/C_6H_9O^+/CH_5O_3S^+$	furfural/1-pentol/methane sulfonic acid	x		x		x
99	$C_6H_{11}O^+/C_5H_7O_2^+/C_4H_3O^+$	cyclohexanone/lactone/maleic anhydride		x	x		x
100	$C_6H_{14}N^+$	cyclohexylamine					
101	$C_6H_{13}O^+/C_5H_9O_2^+/C_4H_5O_3^+$	hexanone/ethylacrylate/succinic anhydride					x
102	$(C_6H_{15}N)H^+$	alkylamine					
103	$(C_6H_{14}O)H^+/(C_5H_{10}O_2)H^+$	diisopropyl ether/propyl acetate/pyruvic acid, methyl ester/methyl butyrate			x		x
104	$C_8H_8^+$	M^+ ion of styrene					
106	$C_4H_{12}NO_2^+$	2-amino-2-methyl-1,3-propanediol or diethanolamine					
107	$(C_7H_6O)H^+$	benzaldehyde					
108	$C_7H_7^+.NH_3/C_7H_{10}N^+$	tropylium-ammonia cluster/benzylamine or ethyl pyridine or methyl aniline				x	
109	$C_6H_5O_2^+/C_7H_9O^+$	quinone/cresols			x		x
110	$C_6H_8NO^+$	aminophenols	x				
111	$C_6H_7NO_2^+$	hydroquinone	x	x	x		x
111	$(C_2H_5SHO_3H)^+$, $[(CH_3)_2SO_3H]^+$	ethylmercaptan or dimethylsulfide					
113	$C_4H_5N_2O_2^+/C_6H_9O_2^+/$ $C_7H_{13}O^+/C_6H_{13}N_2^+$	maleic hydrazide/sorbic acid/ cycloheptanone/triethylenediamine					x

TABLE 2.3-2 (continued)

M/Z	ASSIGNMENTS	COMMENTS	SITES 1	2	3	4	5
115	$(C_7H_{14}O)H^+$	2-heptanone					
116	$(C_5H_9NS)H^+/C_9H_8^+$	isobutyl thiocyanate/indene					x
117	$(C_7H_{16}O)H^+/(C_6H_{12}O_2)H^+$	heptanol and/or butylacetate					
118	$C_6H_{16}NO^+$	2-diethylaminoethanol	x		x		x
119	$C_4H_7O_2S^+/C_8H_7O^+/$ $C_6H_{15}O_2^+$	3-sulfolene/benzofuran cellosolve (2-butoxyethanol)			x		
120	$C_5H_{14}NO_2^+$	2-amino-2-ethyl-1,3-propanediol					
121	$C_5H_{13}O_3^+/C_8H_9O^+$	methyl carbitol/acetophenone					
122	$C_8H_{12}N^+$	N.I.					
123	$C_8H_{11}O^+/C_7H_7O_2^+$	xylenol, phenethyl alcohol/benzoic acid					x
124	$C_6H_6NO_2^+$	nitrosophenol					
125	$C_8H_{13}O^+$	N.I.					x
126	$C_8H_{16}N^+(?)$	coniceine (?)					
127	$C_3H_7N_6^+$ or $C_6H_7O_3^+$	melamine or pyrogallol		x	x		x
128	$C_5H_6NOS^+$	pyrithione					
129	$C_7H_{13}O_2^+/C_8H_{17}O_2^+$	n-butyl acrylate/ethyl amyl ketone or hexyl methyl ketone			x		
130	$C_6H_{12}NS^+$	isoamyl thiocyanate					
131	$C_7H_{15}O_2^+/C_8H_{19}O^+$	ester/alcohol or ether					x
132	$C_9H_{10}N^+$	skatole					
133	$C_9H_9O^+/C_6H_{13}O_3^+$	cinnamaldehyde, 2,2,dimethyl-1, 3-dioxolane-4-methanol or 2,5-tetrahydrofurandimethanol	x		x	x	x
134	N.I.	N.I.					
135	$C_6H_{15}SO^+$	hexylmercaptan or dipropyl sulfide derivatives					
136	$C_7H_6NS^+$	benzothiazole					
137	$C_8H_9O_2^+/C_9H_{13}O^+$	esters/alcohols, ethers					
138	$C_8H_{12}NO^+$	phenylethanolamine					
139	$C_8H_{11}O_2^+/C_6H_7N_2O_2^+/$ $C_4H_{11}O_3S^+$	cresols/nitroanilines/ 2-(ethylsulfonyl) ethanol	x		x	x	x
140	$C_3H_{10}NO_3S/C_6H_6NO_3^+$	n-methyltaurine/nitrophenols					
141	$C_6H_{13}N_4^+$	methenamine (?)					
142	$C_8H_{16}NO^+$ (?)	n-acetylcyclohexylamine (?)					
143	$C_8H_{15}O_2^+$	cyclohexane carboxylic acid, methyl ester					
144	$C_{10}H_{10}N^+$	naphthylamine					
145	$C_6H_9O_4^+/C_8H_{17}O_2^+/$ $C_{10}H_9O^+$	fumaric acid, dimethyl ester or lactide/ ester compound/naphthol			x		x
146	$C_9H_8NO^+$	8-hydroxyquinoline					
147	N.I.	N.I.					
148	$C_8H_6NO_2^+$ (?)	pthalimide (?)				x	
149	$C_8H_5O_3^+$	pthalic anhydride		x	x		x
150	$C_6H_{16}NO_3^+$	triethanolamine					
151	$C_6H_{15}O_4^+$	triethylene glycol					
152	$C_8H_{10}NO_2^+$	acetaminophen		x			
153	$C_8H_9O_3^+$	cresotic acids					
154	$C_7H_8NO_3^+$	amino salicylic acid					
155	$C_7H_7O_2S^+/C_4H_{13}FN_2OP^+/$ $C_{10}H_{19}O^+$	Thiosalicylic acid/Dimefox/-Terpineol/citronellal					
156	NI	NI			x		
157	$C_{10}H_{21}O^+$	citronellol, menthol or rhodinol	x		x		
158	$C_{10}H_{24}N^+$	Diisoamylamine					
159	$C_6H_7O_3S^+$	benzene sulfonic acid					
160	$C_6H_{10}NO_2S^+$	citiolone					
161	NI	NI			x		
162	NI	NI					
163	$C_8H_{19}SO^+$	octyl mercaptan or dibutylsulfide derivatives					
164	$C_6H_{14}NO_4^+$	2-Nitro-2propyl-1,3- propanediol	x	x			
165	$C_8H_9N_2O_2^+/C_{10}H_{13}O_2^+/$ $C_{11}H_{17}O^+$	phthalamide/ethylphenyl acetate/ Jasmone					
166	$C_{10}H_{16}NO^+$	(aminopropyl) benzyl alcohol					
167	$C_9H_{11}O_3^+/C_9H_{15}N_2O^+$	ethyl salicylate or ethyl vanillin/ 5-amino-2-butoxypyridine					
168	$C_{12}H_{10}N^+$	carbazole					
169	$C_8H_9O_4^+$	dehydroacetic acid			x		
170	$(C_{12}H_{11}N)H^+$	diphenylamine					
171	$C_{12}H_{11}O^+$	phenylphenol					
172	$C_7H_{11}ClN_3^+/C_8H_{18}N_3O^+$	crimidine/2-heptanone, semicarbazone					
173	$C_6H_9N_2O_2S^+/C_{10}H_{21}O_2^+$	Porofor BSH/octyl acetate					

TABLE 2.3-2 (continued)

M/Z	ASSIGNMENTS	COMMENTS	SITES 1	2	3	4	5
174	$C_6H_8NO_3S^+$	sulfanilic acid					
175	$C_7H_{11}O_5^+$	adipic acid, dimethyl ester or dimethoxane					
176	$C_6H_7FNO_2S^+$	sulfanilyl fluoride					
177	$C_9H_{21}SO^+$	nonylmercaptan derivative					
178	$C_{10}H_{12}NO_2^+$	acetoacetanilide					
179	$C_8H_{19}SO_2^+$	octylmercaptan or dibutyl sulfide derivative					
180	$C_{10}H_{14}NO_2^+$	IPC					
181	$C_{10}H_{13}O_3^+$	2-phenoxyethanol acetate			x		x
182	$C_{12}H_{24}N^+$	dicyclohexylamine					
183	$C_6H_{17}FN_2OP^+$ /$C_{11}H_{19}O_2^+$/ $C_6H_{15}O_6^+$	mipafox/geraniol, formate/sorbitol					
184	$C_4H_{11}NO_3PS^+$	acephate					
185	$C_{12}H_{13}N_2^+$	benzidine					
186	$C_{12}H_{28}N^+$	tributylamine					
188	NI	NI					
190	$C_{12}H_{16}NO^+(?)$	benzoylpiperidine, or ethyl crotonanilide(?)					
192	$C_{12}H_{18}NO^+/C_{13}H_{22}N^+$	N,N-diethyl-m-toluamide/2,6-Di-tert butylpyridine					
193	$C_{13}H_{21}O^+/C_{12}H_{17}O_2^+$	ionone/isoamyl benzoate					
194	$C_{11}H_{16}NO_2^+$	isobutyl-p-aminobenzoate		x			
196	$C_{11}H_{17}NS^+$	1-naptholisothiocyanate					
197	$C_{11}H_{14}ClO^+/C_{12}H_{20}O_2^+$	dowicide/geraniol, acetate or linalyl acetate					
198	$C_{13}H_{12}NO^+$	benzanilide					
199	$(C_{12}H_{10}N_2O)H^+$	N-nitrosodiphenylamine					
201	$C_6H_5N_2O_6^+$	2,4-dinitroresorcinol					
202	$C_{12}H_{12}NO_2^+$	carbaryl					
203	$C_{10}H_{19}O_4^+$	ethyl adipate/hexyleneglycol, diacetate					
204	$C_9H_{18}NO_2S^+/C_{10}H_{22}NOS^+$	Lethane/pebulate					
206	NI	NI					
208	$C_{12}H_{18}NO_2^+$	promecarb					
214	$C_{13}H_{12}NO_2^+$	salicylanilide	x				
217	$C_{11}H_{21}O_4^+$	esters					
218	NI	NI					
219	$C_7H_7O_6S^+$	sulfosalicylic acid					
220	NI	NI					
221	$C_4H_8Cl_2O_4P^+/C_{11}H_9O_5^+$ /$C_{15}H_{25}O^+SO^+$	Dichlorvos/Purpurogallin/DBMC or santalol or butylated hydroxytoluene					
222	$C_{12}H_{16}NO_3^+/C_{13}H_{20}NO_2^+$	carbofuran/bufencarb					
223	$C_{10}H_{23}O_3S^+$	decylmercaptan or dipentyl sulfide derivatives					
225	$C_{10}H_9O_4S^+/C_7H_{18}O_6P^+$	cassella's acid or napthol sulfonic acid/mevinphos/					
226	$C_{13}H_{12}N_3O^+$	Tinuvin P,					
234	NI	NI					
235	$C_{13}H_{19}N_2O_2^+/C_{17}H_{15}O^+$ $C_8H_{16}N_2O_4P^+/C_{10}H_{17}N_2OS_2^+$	lenacil/dibenzalacetone/ O,O,diethyl-O-(3-methyl-5-pyrazolyl)phosphate or Quinomethionate					
240	$C_{10}H_{10}NO_4S^+/C_{16}H_{17}NO^+$	amino-napthol-sulfonic acid/ diphenamid					
246	$C_{13}H_{16}N_3O_2^+$	pyrolan					
248	NI	NI					

A P P E N D I X 3

PROFILE OF DETECTED CHEMICALS, USES, TOXICITY AND TLV'S

CHEMICALS DETECTED IN THE POSITIVE ION MODE - 3A

CHEMICALS DETECTED IN THE NEGATIVE ION MODE - 3B

REFERENCES SITED

1. Jan. 1/76 issue of 29CFR 190-OSHA Standards

2. NIOSH/OSHA Pocket Guide to Chemical Hazards; DHEW (NIOSH) Publication No. 78-210.

3. The Merck Index, 9th Edition. Published by Merck & Co. Inc. 1976. Printed in U.S.A. Martha Windholz, Editor.

4. ACGIH, 1980. American Conference of Governmental Industrial Hygienists ISBN: 0-936712-29-5.

5. Karel Verschueren, 'Handbook of Environmental Data on Organic Chemicals'. Van Nostrand Reinhold Co; New York, N.Y., 1977.

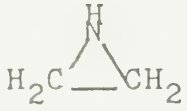
6. Hazardous Chemicals Data Book. Environmental Health Review No. 4, 1980. Edited by G. Weiss, New Jersey, U.S.A.

7. Pesticide Manual Jan., 1977 edited by H. Martin and Charles R. Worthing.

8. Pesticides Safety Handbook. Prepared by Pesticides Control Section, Pollution Control Branch, Ontario Ministry of the Environment, Oct. 1979.

Appendix 3A
Catalog of chemicals with generic and chemical names and structures, uses, and toxicity information.

POSITIVE MODE

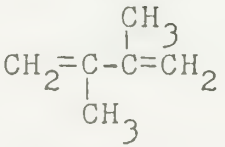
M/Z	COMPOUND	SYNONYM	STRUCTURE	USES	TOXICITY	TLV
30	methane	marsh gas/methyl hydride	CH_4	constituent of illuminating and cooking gas; in the manufacture of hydrogen, hydrogen cyanide, ammonia, acetylene, formaldehyde (3)	simple asphyxiant (3)	suggested: 10,000 ppm (5)
32	methylamine	methanamine	CH_3NH_2	in tanning and in organic syntheses (3)	irritating to eyes, skin & respiratory tract (3)	10 ppm (1)
44	ethylenimine	azacyclopropane		in the manufacture of triethylenemelamine (3)	FDA has declared this substance a carcinogen. Strongly irritating to eyes, skin & mucous membranes. Can be a skin sensitizer. (3)	0.5 ppm (1)
46	dimethyl-amine	N-methyl methanamine	$(CH_3)_2NH$	as accelerator in vulcanizing rubber, tanning, manuf. detergent soaps, or attracting boll weevils to exterminate them (3)	irritating to skin and mucous membranes	10 ppm (1)
46	ethylamine	ethanamine	$C_2H_5NH_2$	In resin chemistry; stabilizer for rubber latex; intermediate for dyestuffs, medicinals; in organic syntheses. (3)	Irritating to skin, mucous membranes, respiratory tract. (3)	10 ppm (1)
48	methoxyamine	O-methylhydroxylamine	CH_3ONH_2	analytical reagent for aldehydes and ketones. (3)	strong irritant (3)	Data not available.
49	methylmercaptan	methanethiol	CH_3SH	Data not available	narcosis, cyanosis, convulsions, pulmonary irritation; respiratory paralysis; headaches, nausea. (2)	10 ppm/ 15 min ceil (20mg/m^3) (2)

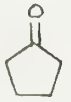
M/Z	COMPOUND	SYNONYM	STRUCTURE	USES	TOXICITY	TLV
56	propionitrile	propane nitrile	CH_3CH_2CN	Data not available	May cause dizziness, rapid respiration, headache, drowsiness, drop in blood pressure & pulse, and unconsiousness, delayed symptoms, chronic exposure may result in eye irritation, loss of appetite, mental deterioration (2)	6 ppm (NIOSH value) (6).
57	acrolein	2-propenal	$CH_2=CHCHO$	manufacture colloidal forms of metals; making plastics, perfumes (3). Also used as an aquatic herbicide (7).	Irritates skin, eyes and mucous membranes. Vapors cause lacrimation. A weak sensitizer; inhalation may cause asthmatic reaction. Inhalation of high conc'ns causes pulmonary edema.	0.1 ppm (1)
58	allylamine	2-propen-1-amine	$CH_2=CHCH_2NH_2$	in the manufacture of mercurial diuretics. (3)	a strong irritant to eyes, mucous membranes, can cause excitement, convulsions, death. (3)	Data not available (6)
59	acetone	2 propanone	CH_3COCH_3	Solvent for fats, oils, waxes, resins, rubber, plastics, lacquers varnishes, rubber cements. (3)	prolonged or repeated topical use may cause erythema, dryness. Inhalation may produce headache, fatigue, excitement. (3)	1000 ppm (2)
60	acetamide	acetic acid amide	CH_3CONH_2	Solvent; solubilizer, plasticizer, stabilizer. Manufacture of methylamine, denaturing alcohol. In organic sytheses. (3)	No skin/eye irritation (6), Carcinogenic (6) Drowsiness, fatigue, nausea, acidosis, skin eruptions may occur upon exposure to cpd. (6)	Not available (6)
60	propanamine	-		no data available	no data available	none available

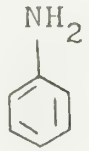
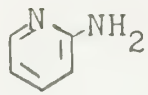
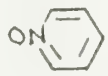
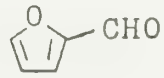
M/Z	COMPOUND	SYNONYM	STRUCTURE	USES	TOXICITY	TLV
61	ethylmethylether	methoxyethane	$C_2H_5OCH_3$	Data not available	No data available	No data available.
61	propyl alcohol	1-propanol	$CH_3(CH_2)OH$	Solvent for resins and cellulose esters. (3)	Mildly irritating to eyes, mucous membranes; depressant action similar to ethyl alcohol (3)	200 ppm (1)
61	methyl formate			Fumigant and larvicide for tobacco, dried fruits, cereals, etc. (3)	inhalation of vapor produces nasal and conjunctival irritation, retching, narcosis, death from pulmonary irritation. (3)	100 ppm (1)
61	ethylenediamine	1,2-ethanediamine	$H_2N(CH_2)_2NH_2$	Solvent for casein, albumin, shellac, and sulfur; emulsifier; stabilizing rubber latex; as inhibitor in antifreeze solutions (3)	because of its caustic nature and irritating properties, can cause nasal irritation, sensitization dermatitis, irritation of the respiratory system. (3)	10 ppm (1)
63	ethylene glycol	1,2-ethanediol	$HOCH_2CH_2OH$	Antifreeze in cooling and heating systems. Solvent in paints, and plastics industries. Softening agent for cellophane. (3)	Constitutes a hazard when ingested, e.g. drinking of antifreeze fluid. Transient stimulation of CNS followed by depression; vomiting, drowsiness, coma, respiratory failure. May proceed to death. (3)	lethal dose: 1.4ml/kg or 100 ml (3)
65	methyl mercaptan derivative		CH_5SO^+	-	-	

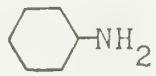
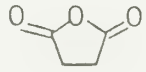
M/Z	COMPOUND	SYNONYM	STRUCTURE	USES	TOXICITY	TLV
67	cyclopentadiene	1,3-cyclopentadiene		manuf resins; in organic syntheses, synthetic alkaloids, camphors. (3)	irritating to the eyes and nose. (3)	75ppm (1)
69	furan	divinylene oxide or furfuran		no data available	vapors are narcotic, can be absorbed through skin (3)	not pertinent
69	pyrazole	1,2-diazole		no data available	no data available	no data available
70	butane nitrile	propyl cyanide or butyronitrile		no data available	highly toxic (3)	P.O.L: 50 ppm (3)
71	crotonaldehyde	trans 2-butenal		in organic syntheses, as solvent in purification of mineral oils, manuf of resins, rubber antioxidants, insecticides (3)	highly irritating to eyes, skin and mucous membranes (3)	2ppm (6)
71	methyl vinyl ketone	3-buten-2-one	$CH_3COCH=CH_2$	commercial starting material for plastics (3)	readily absorbed through skin causing general poisoining of the organism. Irrit to mucous membranes and respiratory tract (3)	data not available (6)
72	hydracrylo-nitrile	3-hydroxy-propanenitrile		solvent for some cellulose esters and many inorganic salts (3)	no data available	no data available
72	acrylamide	propenamide	$CH_2=CHCONH_2$	no data available	highly toxic and irritant. Causes CNS paralysis. Can be absorbed through unbroken skin (3)	0.3 mg/m3 (4)

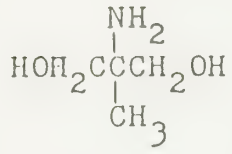
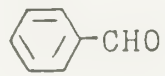
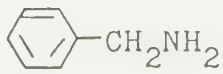
M/Z	COMPOUND	SYNONYM	STRUCTURE	USES	TOXICITY	TLV
74	butylamine	1-amino-butane	$CH_3(CH_2)_3NH_2$	intermediate for pharmaceuticals, dyestuffs rubber chemicals, emulsifying agents, insecticides, synthetic tanning agents (3)	potent skin, eye, mucous membrane irritant. Direct skin contact causes severe primary irritation and blistering (3)	5ppm (1)
74	diethylamine	n-ethylethanamine	$(C_2H_5)_2NH$	in the rubber and petroleum industry; in resins, dyes pharmaceuticals (3)	may be irritating to skin, mucous membranes (3)	25ppm (1)
74	dimethyl-formamide	DMF	$(CH_3)_2NCH$ (=O)	solvent for liqs and gases. In the synthesis of organic compounds, solvent for orlon and similar polyacrylic fibers. (3)	vapour harmful. Irritant to eyes, skin and mucous membranes. Liver injury has been produced in expt'l animals by prolonged inhalation of 100ppm (3)	100ppm (1)
75	dimethyl-nitrosoamine			no data available	no data available	
75	diethylether			no data available	no data available	
75	t-butanol	3-butanol		not data available	no data available	
77	propylene glycol	1,2-propandiol	$CH_3CH(OH)CH_2OH$	as non-toxic antifreeze in breweries and dairy establishments. In the manuf of synthetic resins as mist to disinfect air (3)	Therap cat: pharmaceutic aid (humectant solvent). Liquid may irritate eyes (3)	not pertinent (6)
77	methyl-cellosolve®	2-methoxyethanol	$HO(CH_2)_2OCH_3$	solvent for low-viscosity cellulose acetate, natural and synthetic resins, and some alcohol-soluble dyes; sealing moisture-proof cellophane, nail polishes, wood stains (3)	may cause anemia, macrocytosis, appearance of young granulocytes in blood; also CNS symptoms. Readily absorbed through skin (3)	25ppm (1)

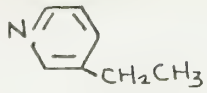
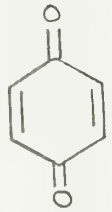
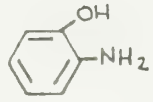
M/Z	COMPOUND	SYNONYM	STRUCTURE	USES	TOXICITY	TLV
77	trimethylene-glycol	1,3-propanediol	$HO(CH_2)_3OH$	no data available	exposure may cause coldness, spastic contraction of muscles, loss of reflexes, coma, death, pulmonary edema, eye irritation. Chronic exposure may cause weakened reflexes. (3)	none available (6)
79	dimethyl sulfoxide	methylsulfoxide or DMSO	CH_3SOCH_3	solvent for acetylene, sulfur dioxide and gases. As paint and varnish remover (3)	slight eye irritation may occur (6)	not available (6)
79	2 mercaptoethanol	nonothioglycol		no data available	no data available	
80	pyridine			as a solvent for anhydrous mineral salts, in organic syntheses, and in analytical chemistry (3)	may cause CNS depression, irriation of skin and respiration tract. Large dose may produce GI disturbances, kidney and liver damage (3)	5ppm (1)
81	pyrazine	1,4-diazine		no data available	no data available	
81	pyridazine	1,2-diazine		no data available	no data available	
81	pyrimidine	1,3-diazine		no data available	no data available	
82	cyclohexane	hexahydrobenzene		solvent for lacquers and resins. Paint and varnish remover. In fungicidal formulations (3)	high concns may act as narcotic, skin irritant (3)	300ppm (1)
82	2,3-dimethyl-1,3-butadiene	diisopropenyl		in manuf of synthetic rubber and polymers (3)	no data available	
81	methylfuran		$C_4H_3OCH_3$	no data available	no data available	not pertinent

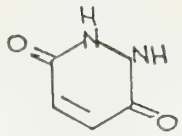
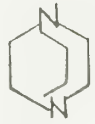
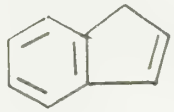
M/Z	COMPOUND	SYNONYM	STRUCTURE	USES	TOXICITY	TLV
85	diketene		$(CH_2=C=O)_2$	monomer is used for the conversion of higher acids into their anhydrides; for acetylation in the manuf of cellulose acetate and aspirin (3)	monomer is a severe pulmonary irritant causing pulmonary edema if inhaled (3)	none available
85	cyclopentanone	ketocylcopentane		no data available	no data available	
87	methylacrylate	2-propenoic acid methyl ester	$CH_2=CHC(=O)-OCH_3$	monomer in manuf of leather finish resins, textile and paper coatings, and plastic films (3)	the monomer is highly irritating to eyes, skin, mucous membranes. Lethargy and convulsions may occur if vapors of monomer are inhaled in high concns. (3)	10ppm(1)
87	methacrylic acid	2-methyl propenoic acid	$CH_2=C(CH_3)-COOH$	manuf of methacrylate resins and plastics (3)	may act as a strong irritant (3)	not pertinent (5)
90	2-amino-2-methyl-1-propanol		$CH_3C(NH_2)(CH_3)CH_2OH$	in synthesis of surface active agents, vulcanization accelerators, pharmaceuticals as emulsifying agent for cosmetic creams and lotions, mineral oil, polishes, cleaning compounds (3)		
90	urethan	carbamic acid ethyl ester	$NH_2C(=O)-OC_2H_5$	molten urethan is a good solvent for various organic materials. As solubilizer and cosolvent for pesticides, fumigants (3)	Therap Cat: antineoplastic (3)	
93	glycerol	1,2,3-propanetriol		as solvent, humectant, plasticizer, sweetener. In manuf of cosmetics, liquers, confectioneries, lubricants, as antifreeze, in shock absorber fluids (3)	Therap Cat: Pharmaceutic aid (humectant;solvent) (3)	

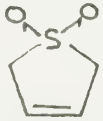
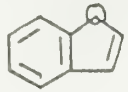
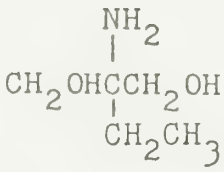
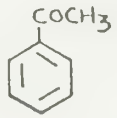
M/Z	COMPOUND	SYNONYM	STRUCTURE	USES	TOXICITY	TLV
94	methylpyridine	picoline		no data available	severe skin & eye irritation, narcosis, headache, nausea, giddiness, vomitting. Chronic exposure may result in occasional vomitting and diarrhea, weight loss and anemia (3)	not available
94	aniline	benzenamine		manuf dyes, medicinals, resins, varnishes, perfumes, shoe blacks, vulcanizing rubber, as solvent	intoxication may occur from inhalation, ingestion, or cutaneous absorption. Acute: cyanosis, methemoglobinemia, vertigo, headache, mental confusion (3)	0.5ppm (1)
95	aminopyridine			manuf. of drugs and dyes (3)	inhalation may cause headaches, dizziness, nausea. Flush extremities and high blood pressure may result from skin adsorption (2)	0.5ppm (2)
96	pyridine-1-oxide			synthetic intermediate (3)	no data available	
97	furfural	2-furancarboxaldehye		in the manuf of furfuralphenol plastics such as durite; in solvent refining of petroleum oils. In the manuf of varnishes; as insecticides, fungicide, germicide (3)	irritates mucous membranes and acts on CNS. Causes lacrimation, inflammation of eyes, irritation of throat, headache (3)	5ppm (2)

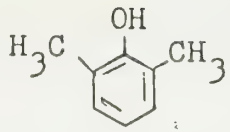
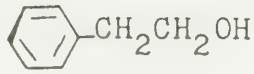
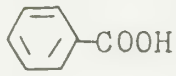
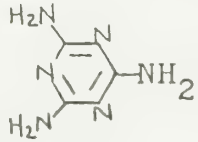
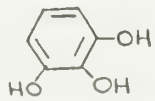
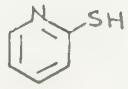
M/Z	COMPOUND	SYNONYM	STRUCTURE	USES	TOXICITY	TLV
97	1-pentol	3-methyl-2-penten-4-yn-1-ol	$HC\equiv CC(CH_3)=CHCH_2OH$	intermediate in Vitamin A synthesis (3)	both isomers tend to polymerize and will explode when heated above above 120° in a sealed bomb tube (3)	none available
97	methanesulfonic acid	methylsulfonic acid	CH_3SO_2OH	as a catalyst in polymerization, alkylation and esterification as a solvent (3)	strong irritant (3)	
99	cyclohexanone			solvent for cellulose acetate, nitrocellulose, natural resins, crude rubber, waxes, fats, DDT. In prod of adipic acid for nylon (3)	irritating to eyes, mucous membranes (3)	50ppm (1)
99	lactone			no data available	no data available	
99	maleic anhydride	2,5-furandione		in organic syntheses, manuf of alkyd-type of resins, dye intermediates, agricultural chemicals, pharmaceuticals (3)	powerful irritant, causes burns. Inhalation can cause pulmonary edema. Avoid contact with skin, eyes (3)	0.25ppm (1)
100	cyclohexylamine	aminocyclohexane		in organic synthesis, manuf insecticides, plasticizers, rubber chemicals, dyestuffs, dry-cleaning soaps (3)	can cause irritation and sensitization. High cocn's cause nausea and narcotic effects (3)	10ppm, 1972 (5)
101	hexanone	methylisobutyl ketone		no data available	200 ppm; eye irritation 400; nasal irritation inhalation: survived: 2,000 ppm, 4hr death: 400 ppm, 4hr (2)	100 ppm (2)
101	succinic anhydride	dihydro-2,5-furandione		no data available	no data available	
101	ethyl acrylate	2-propenoic acid ethyl ester		in manuf. of water emulsion paint vehicles, textile and paper coatings leather finish resins and adhesives (3)	monomer is highly irritating to eyes, skin, mucous membranes. Lethargy and convulsions may occur if vapors of monomer are inhaled in high concn's. (3)	25 ppm (1)

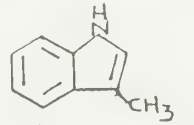
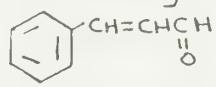
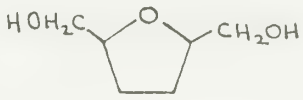
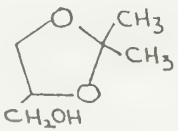
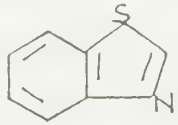
M/Z	COMPOUND	SYNONYM	STRUCTURE	USES	TOXICITY	TLV
103	diisopropylether			no data available	no data available	
103	methyl butyrate	butanoic acid methyl ester		manuf. artificial rum and fruit essences (3)	no data available	
103	propyl acetate			manuf. flavors, perfumes. Solvents for resins, cellulose derivatives and plastics. (3)	may be irritating to skin, mucous membranes, and in high concn's narcotic (3)	200 ppm (1)
104	styrene	ethenylbenzene		manuf. plastics; synthetic rubber; resins; insulator (3)	may be irritating to eyes mucous membranes, and in high concns, narcotic (3)	100 ppm (1)
106	2-amino-2-methyl-1,3-propanediol			in synthesis of surface active agents. As emulsifying agent for cosmetic creams and lotions, mineral oil and paraffin wax, polishes, cleaning compounds (3)	no data available	
106	diethanolamine	2,2'-Iminobis ethanol	$(HOCH_2CH_2)_2NH$	as rubber chemicals intermediate, in surface active agents used in textile specialities, herbicides, petr demulsifiers. In various agricultural chemicals, cosmetics (3)	Vapors may cause moderate irritation, skin contact may cause first-degree burns on short exposure and may cause secondary burns on long exposure (6)	not pertinent
107	benzaldehyde	benzenecarbonal		manuf. of dyes, perfumery, cinnamic and mandelic acids; as solvent; in flavors (3)	narcotic in high concn's May cause contact dermatitis. (3)	not available (6)
108	benzylamine	α-aminotoluene		in organic syntheses (3)	highly irritating to skin, mucous membranes (3)	

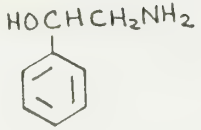
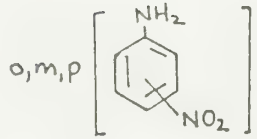
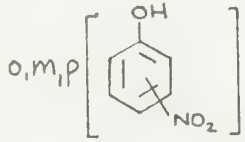
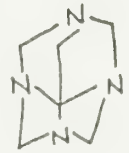
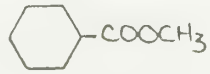
M/Z	COMPOUND	SYNONYM	STRUCTURE	USES	TOXICITY	TLV
108	ethyl pyridine			no data available	no data available	
108	methyl aniline	N-methylbenzenamine		biodegradation: decomposition by a soil microflora (3)	severe toxic effects: 40 ppm, 60 min. Symptoms of illness, 10 ppm. Unsatisfactory, 5 ppm	5 ppm 1974 (5)
109	quinone	2,5-cyclohexadiene-1,4 -dione		oxidizing agent; in photography; manuf. dyes; tanning hides; strengthening animal fibers (3)	can cause dermatitis, erythema, formation of papules and vesicles. Vapors acting on eye can cause conjunctivitis and corneal ulceration (3)	0.1 ppm (1)
109	cresols			as disinfectant like phenol; also as a solvent (3)	inhalation can cause depression, resp. failure; dyspnea (3)	5ppm (2)
110	aminophenols	hydroxy aniline		manuf of azo and sulfur dyes; dyeing furs and hairs (3)	no data available	
111	hydroquinone			as photographic reducer and developer (3)	dermatitis can result from skin contact. Staining and opacification of cornea occur in workers exposed for prolonged periods to concn's of vapor not high enough for prod of systemic effects (3)	2mg/m^3 (2)

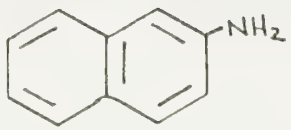
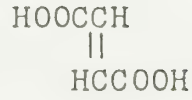
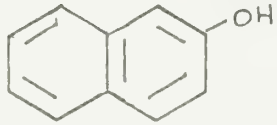
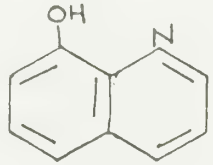
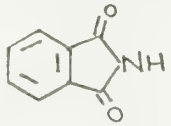
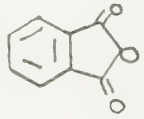
M/Z	COMPOUND	SYNONYM	STRUCTURE	USES	TOXICITY	TLV
113	maleic hydrazide	1,2-dihydro-3,6-pyridazinedione		as photographic reducer and developer (3)	Inhalation of dust causes irritation of nose & throat. Contact with skin or eyes causes irritation (3)	Not available (6)
113	sorbic acid	2,4-hexadienoic acid		mold and yeast inhibitor. Fungistatic agent for foods, especially cheeses. To improve characteristics of drying oils. (3)	no data available	
113	cycloheptanone	ketoheptamethylene		no data available	no data available	
113	triethylenediamine	1,4-diazabicyclo (2.2.2)octane		catalyst in making urethane foams (3)	no data available	
115	2-heptanone	methylamyl ketone	$CH_3(CH_2)_4COCH_3$	in perfumery as constituent of artificial carnation oils; as industrial solvent (3)	no data available	100 ppm, 1974 (5)
116	isobutyl thiocyanate	isobutyl sulfocyanate		no data available	no data available	
116	indene	indonapthene		found in tars from coal, lignite and crude petroleum. Used in paint and coating mfg. chemical synthesis intermediate (3)	Slight skin & eye irritation. Irritation of mucuous membranes & lungs, pulmonary edema. Chronic exposure may cause dermatitis, liver & kidney damage (6)	10 ppm, $45mg/m^3$ (6)
117	heptanol	n-heptyl alcohol		no data available	low toxicity, liquid may irritate eyes (6)	not available (6)
117	butylacetate	acetic acid 1,1-dimethylethyl ester	$CH_3\overset{O}{\overset{\|}{C}}-OC(CH_3)_3$	as gasoline additive (3)	mild eye and nose irritation : 200-300 ppm. unsatisfactory >200 ppm symptoms of illness: 500ppm severe toxic effects: 2,000 ppm, 60 min. (5)	200 ppm (1)

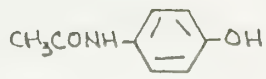
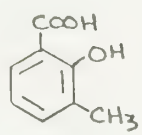
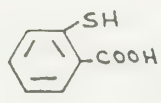
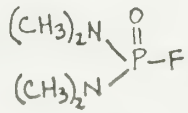
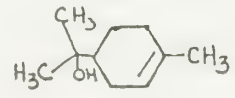
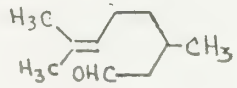
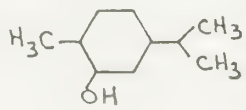
M/Z	COMPOUND	SYNONYM	STRUCTURE	USES	TOXICITY	TLV
118	2-diethyl amino ethanol	2,hydroxy triethylamine	$(C_2H_5)_2NCH_2CH_2OH$	no data available	severe skin & eye irritation, Dermatitis, weight loss, slight increase in clotting time. (3)	10 ppm (6)
119	3-sulfolene	2,5-dihydrothiophene 1,1-dioxide		organic solvent (3)	no data available	
119	benzofuran	coumarone		manuf. of coumarone-indene resins (3)	no data available	
119	butyl cellosolve®	2-butoxyethanol		solvent for nitrocellulose resins, grease, oil, albumin; dry cleaning (3)	Inhalation can result in kidney damage; brain damage eye irritation. (3)	50 ppm (1)
120	2-amino-2ethyl 1,3propanediol			in synthesis of surface active agents, pharmaceutical. As emulsifying agent for cosmetic creams and lotions, mineral oil, paraffin wax, polishes, dry cleaning compounds (3)	no data available	
121	methyl carbitol®	2-(2-methoxyethoxy) ethanol		solvent for nitrocellulose, lacquers and dopes; in varnish removers, cleaning solutions, dye baths. (3)	no data available	
121	acetophenone	1-phenyl ethanone		in perfumery, catalyst for polymerization of olefins, in organic synthesis, esp. as a photosensitizer. (3)	Therap Cat: Hypnotic (3) Notoxicity expected from inhalation or ingestion except slight narcotic effect. Liquid can cause eye & skin irritation on contact. (6)	Not available (6)

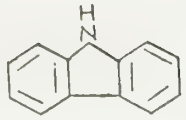
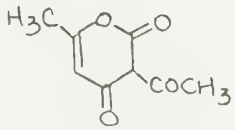
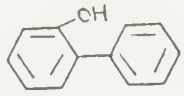
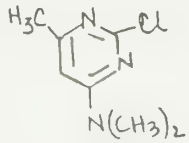
M/Z	COMPOUND	SYNONYM	STRUCTURE	USES	TOXICITY	TLV
123	xylenol	dimethylphenol		for the prep. of coal tar disinfectants; manuf. of artificial resins (3)	Vapor irritates eyes, nose & throat, and is readily absorbed through mucous membranes & lungs, producing general toxic symptoms (weakness, dizziness, headache, difficult breathing, twitching) (6)	45 ppm (6)
123	phenethyl alcohol	2-phenyl ethanol		in flavors and perfumery (3)	Therap Cat: Pharmaceutic aid (antimicrobial agent) (3)	
123	benzoic acid	benzene carboxylic acid		preserving foods, fats, fruit juices, alkaloidal sol'ns. in dyes; for curing tobacco (3)	Mild irritant to skin, eyes and mucous membranes (6)	Not pertinent (6)
124	nitrosophenol			no data available	can cause skin irritation, sensitization. (3)	
126	coniceine			no data available	no data available	
127	melamine	1,3,5-triazine-2,4,6-triamine		forms synthetic resins with formaldehyde (3)	no data available	
127	pyrogallol	1,2,3 benzene triol		developer in photography, as mordant for wool, staining leather, process engraving; manuf. various dyes, furs, hairs (3)	Ingestion may cause severe G.I. irritation, renal and hepatic damage, hemolysis convulsions, circulatory collapse, death (3)	
128	pyrithione	1-hydroxy-2(1H)-pyridinethione		fungicide, bacteriacide (3)	Therap Cat: Zinc deriv. as antibacterial; topical antifungal; anti seborrheic (3)	

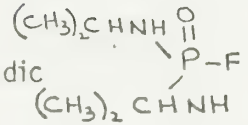
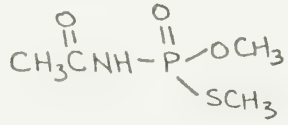
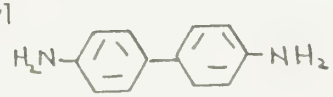
M/Z	COMPOUND	SYNONYM	STRUCTURE	USES	TOXICITY	TLV
129	n-butyl acrylate	2-propenoic acid butyl ester	$CH_2{=}CHC(=O)-OC_4H_9$	the monomer in the manuf. of polymers and resins for textile and leather finishes, paint formulations. (3)	Vapor is irritating when breathed at high concentrations. Contact with liquid causes irritation of skin & burning of eyes (6)	Data Not available (6)
129	ethyl amyl ketone	5-methyl-3-heptanone		solvent for nitrocellulose -alkyd nitrocellulose-maleic, and vinyl resins. (3)	narcotic in high concentrations (3)	25 ppm (1)
129	hexyl methyl ketone	2-octanone	$CH_3(CH_2)_5C(=O)CH_3$	no data available	no data available	not pertinent
130	isoamylthiocyanate	isoamyl sulfocyanate	$(CH_3)_2CH(CH_2)_2SCN$	no data available	no data available	
132	skatole	3-methyl-1H-indole		constituent of beetroot nectandra, wood and coal tar (3)	no data available	
133	cinnamaldehyde	3-phenyl-2-propenal		in flavor and perfume industry (3)	no data available	
133	2,5-tetrahydrofuran-dimethanol	THF glycol		solvent, softener, humectant. In the synthesis of plasticizers, resins, surfactants, agricultural chemicals (3)	highly irritating to eyes skin, mucous membranes (3)	
133	2,2-dimethyl-1,3-dioxolane -4-methanol			versatile solvent and plasticizer (3)	no data available	
135	hexylmercaptan derivative		$C_6H_{15}SO^+$	no data available	no data available	
135	dipropylsulfide		$C_3H_7-S-S-C_3H_7$	no data available	no data available	
136	benzothiazole			photographic dye mfg; rubber chemicals mfg. (3)	no data available	

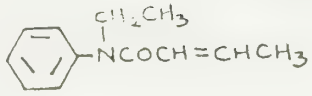
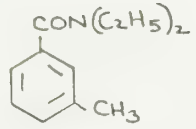
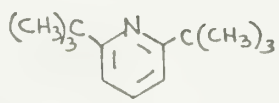
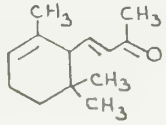
M/Z	COMPOUND	SYNONYM	STRUCTURE	USES	TOXICITY	TLV
138	phenylethanolamine			free base as a stopping agent during polymerization of styrene-butadiene rubber; in hardening of waxes. Intermediate in the manuf. of pressor amines. (3)	no data available	
139	nitroanilines			dyestuff intermediate (3)	Highly toxic; absorbed through skin. Avoid breathing dust. Acute exposure can cause methoglobinemia, cyanosis (5)	1 ppm, 1974 (5)
139	2-ethyl sulfonyl ethanol			intermediate for pharmaceuticals, plasticizers, solvents. Humectant. Antistatic agent for synthetic fibers and fabrics (3)	no data available	
140	methyltaurine	2-methylamino ethane sulfonic acid	$CH_3NH(CH_2)_2SO_3H$	intermediate in the manuf. of surface active agents (3)	no data available	
140	nitrophenols			manuf. of many important compounds; as indicator in 2% alcohol solutions (3)	Moderate eye & mucous membrane irritation, C.N.S. depressant. Inhalation or ingestion causes headache, drowsiness, nausea & cyanosis Can be absorbed through skin to give same symptoms as for inhalation. (6)	None available
141	methenamine	1,3,5,7-tetrazatricyclo [3.3.1.$1^{3.7}$]-decane		in adhesives, coatings, and sealing compounds; as dye fixative; as stabilizer for lubricating and insulating oils (3)	Therap Cat: antibacterial (urinary) (3)	
142	n-acetyl cyclohexylamine			no data available	no data available	
143	cyclohexane carboxylic acid, methyl ester			solubilizer for vulcanized rubber, clarifier for mineral oil; in insecticide formulations. (3)	no data available	

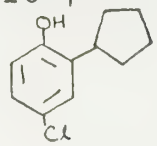
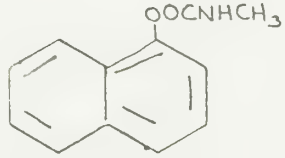
M/Z	COMPOUND	SYNONYM	STRUCTURE	USES	TOXICITY	TLV
144	napthylamine			manuf. dyes (3)	harmful dust and vapor. The FDA has declared this substance a carcinogen. (3) Unsatisfactory >.01 mg/m^3 (5)	Not available (6)
145	fumaric acid, dimethyl ester	(E)-butenedioic acid		substitute for tartaric acids in beverages and baking powders. As an antioxidant. Manuf. polyhydric alcohols, synthetic resins. As mordant in dyeing. (3)	no data available	
145	napthol	hydroxy napthalene		manuf. dyes, perfumes, intermediates, the largest use is probably in making antioxidants for the synthetic rubber industry. (3)	Local action may produce peeling of the skin which may be followed by persistent pigmentation. Ingestion of large quantities may cause nephritis, lens opacity, vomitting and diarrhea abdominal pain, circulatory collapse, death. (3)	None available (6)
146	8-hydroxyquinoline	8-quinolinol		as fungistat, also as a chelating agent (3)	Carcinogen stimulation of CNS, digestive system irritation, eye irritation (6)	None available (6)
148	pthalimide	1 H-Isoindole-1,3 (2H)-dione		no data available	no data available	
149	pthalic anhydride	1,3-isobenzo furandione		manuf. phthaleins, phthalates, benzoic acid, synthetic indigo, artificial resins (glyptal) (3)	Vapor is moderately irritating, skin contact may cause first degree burns on short exposure, and secondary burns on long exposure (6)	2 ppm (1)

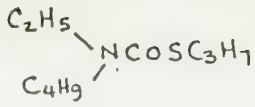
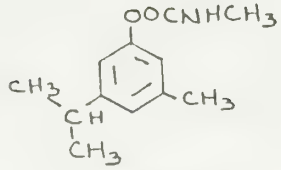
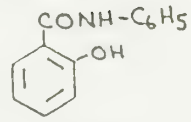
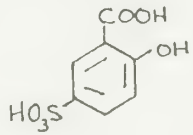
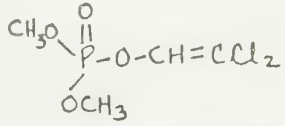
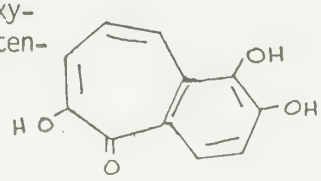
M/Z	COMPOUND	SYNONYM	STRUCTURE	USES	TOXICITY	TLV
150	triethanolamine	trihydroxytriethylamine	$(HOCH_2CH_2)_3N$	intermediate in manuf. of surface active agents, textile specialties, waxes, polishes, herbicides, petroleum demulsifiers, toilet goods. Solvent for shellac, dyes; manuf. synthetic resins. (3)	liquid may irritate eyes and skin (6)	Not pertinent (6)
151	triethylene glycol	triglycol	$CH_2OCH_2CH_2OH$ $CH_2OCH_2CH_2OH$	in various plastics to increase pliability; in air disinfection (3)	very low acute and chronic toxicity (5)	Not pertinent (6)
152	acetaminophen	4'-hydroxy acetanilide		manuf. azo dyes, photographic chemicals (3)	Therap Cat: analgesic antipyretic (3)	
153	cresotic acid			in manuf. of dyes (3)	Toxicity similar to salicylic acid. (i.e. absorption of large amounts can cause vomiting, abdominal pain, inc. resp., acidosis. May also cause skin rashes. (3)	
155	thiosalicylic acid	2-mercapto benzoic acid		manuf. thioindigo dyes (3)	no data available	
155	Dimefox	tetramethyl phosphorodiamidic fluoride		pesticide (3)	a highly toxic cholinesterase inhibitor, symptoms similar to parathion, q.v. (3)	Oral LD50= 1-2mg/kg (8)
155	terpineol	α,α,4-trimethyl-3-cyclohexene-1-methanol		perfumes; denaturing fats for soap manufacture (3)	Therap Cat: antiseptic (3)	
155	citronellal	3,7-dimethyl-6-octenal		in soap perfumes; insect repellant (3)	no data available	
157	menthol	5-methyl-2- (1-methylethyl) cyclohexanol		in liquers, confectionery, perfumery, cigarettes, cough drops, and nasal inhalers (3)	Therap Cat: topical antipruritic (3)	
157	citronellol	3,7,-dimethyl-6-octene 1-ol		in perfumery (3)	no data available	

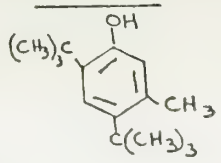
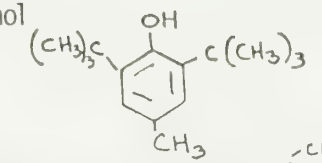
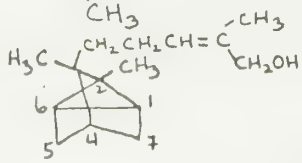
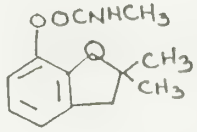
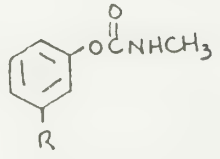
M/Z	COMPOUND	SYNONYM	STRUCTURE	USES	TOXICITY	TLV
167	5-amino-2-butoxy pyridine			no data available	no data available	
168	carbazole	9-azafluorene		important dye intermediate. Used in making photographic plates sensitive to ultraviolet light (3)	no data available	
169	dehydroacetic acid			in organic syntheses; as plasticizer, compatible with nitro- , cellulose, polystyrene methacrylate, vinylite resins; as fungicide and bacteriacide; in antienzyme toothpastes (3)	causes impaired kidney function. Large doses can cause vomitting, ataxia, convulsions (3)	
170	diphenylamine	N-phenylbenzene amine		manuf. dyes; stabilizing nitrocellulose explosives and celluloid. In anal. chem for the detection of NO_3, ClO_3 and other oxidizing substances (3)	may be irritating to mucous membranes. . Overexposure, including ingestion of solid or skin contact, may cause fast pulse, hypertension and bladder trouble. Contact with dust irritates eyes (6)	10 mg/m^3 (6)
171	phenyl phenol	O-hydroxybiphenyl		as intermediate in the manufacture of resins; also in the rubber industry (3)	no data available	
172	crimidine	2-chloro-N,N,6-trimethyl -4-pyrimidinamine		rodenticide (3)	may cause serious CNS damage leading to fatal convulsions (3)	
172	2-heptanone semicarbazone			in perfumery as constituent of artificial carnation oils; as industrial solvent (3)	no data available	

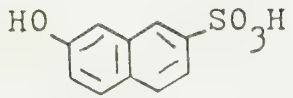
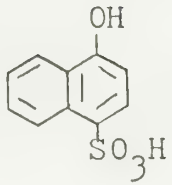
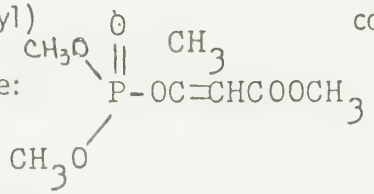
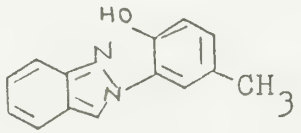
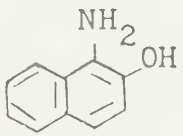
M/Z	COMPOUND	SYNONYM	STRUCTURE	USES	TOXICITY	TLV
181	2-phenoxyethanol acetate			fixative for perfumes in org. synthesis; as bacteriacide in conjunction with quaternary ammonium cpds; as insect repellant (3)	no data available	
182	dicyclohexylamine	N-cyclohexyl cyclohexanamine		in organic synthesis, manufacture insecticides, plasticizers, corrosion inhibitors, rubber chemicals, dyestuffs, emulsifying agents, dry-cleaning soaps, acid gas absorbents (3)	a skin irritant and possible sensitizer (3)	20 ppm (suggested) (6)
183	Mipafox	N,-N'-Bis(1-methyl ethyl) phosphorodiamidic fluoride		insecticide (3) (3)	cholinesterase inhibitor	
183	geraniol formate			as constituent of artificial neroli oil and of artificial orange blossom oil. (3)	no data available	
183	sorbitol	D-glucitol	$CH_2OH(HCOH)_4CH_2OH$	in manufacture of sorbose, ascorbic acid, propylene glycol, synthetic plasticizers and resins; as moisture conditioner on printing rolls, in leather, tobacco. In writing inks. In antifreeze mixtures with glycerol or glycols. (3)	Therap Cat: Pharmaceutic aid (sweetening agent; tablet excipient). (3) Hot liquid will burn skin. (6)	Not pertinent (6)
184	acephate	acetylphosphoramidothioic acid O,S-dimethyl ester		contact and systemic insecticide (3)	No teratogenic effects noted in rats and rabbits, except for slight moderate effects on cholinisterase depression (7)	
185	benzidine	4,4'-diamino biphenyl		manufacture dyes; as a reagent for H_2O_2 in milk and for detection of blood. (3)	FDA has declared this substance and its salts as carcinogens. (3)	

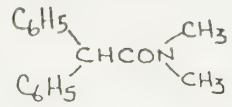
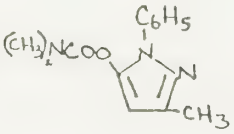
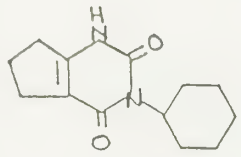
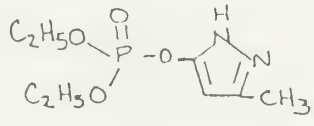
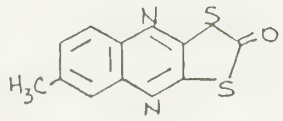
M/Z	COMPOUND	SYNONYM	STRUCTURE	USES	TOXICITY	TLV
186	tributylamine	N,N-dibutyl-1-butanamine	$[CH_3(CH_2)_3]_3N$	no data available	causes CNS stimulation, skin irritation, sensitization. (3)	P.O.L. 10 ppm
190	benzoylpiperidine			no data available	no data available	
190	ethylcrotonanilide			no data available	Therap Cat: antipruritic (3)	
192	N,N-diethyl-m-toluamide	N,N-diethyl-3-methylbenzamide		insect repellent (3)	Irritant to eyes, mucous membranes, but not to skin. Ingestion can cause CNS disturbances. (3)	
192	2,6-di-tert-butylpyridine			has been proposed as an additive for lubricating oil, gasoline and for stabilizing Cl-containing polymers. (3)	no data available	
193	ionone	α-cyclocitrylidene acetone		in perfumery (3)	may cause allergic reactions (3)	
193	isoamylbenzoate			in perfumery and cosmetics (3)	no data available	
194	isobutyl-p-aminobenzoate			no data available	no data available	

M/Z	COMPOUND	SYNONYM	STRUCTURE	USES	TOXICITY	TLV
196	1-naphthyl isothiocyanate	1-isothiocyanato naphthalene	$C_{10}H_7N=C=S$	has been used with pyrethrum as insecticide (3)	hepatotoxic; may cause dermatitis (3)	
197	dowicide	4-chloro-2-cyclo pentylphenol		germicide (3)	no data available	
197	geraniol acetate			no data available	no data available	
197	linalyl acetate	3,7-dimethyl-1,6-octadien-3-yl acetate		in perfumery (3)	no data available	
198	benzanilide	N-phenylbenzamide		manufacture dyes and perfumes (3)	no data available	
199	nitrosodiphenyl amine			accelerator in vulcanizing rubber (3)	no data available	
201	2,4 dinitro resorcinol	2,4-dinitro-1,3- benzene diol		for dyeing fabrics mordanted with iron. As a reagent for Co and for Fe (3)	no data available	
202	carbaryl	1-naphthalenol methyl carbamate		contact insecticide (3)	Data not available (6)	5mg/m^3 (6) oral LD50 = 400-850 mg/kg (8)
203	ethyl adipate	hexanedioic acid diethyl ester		no data available	no data available	
203	hexylene glycol diacetate	2-methyl-2,4-pentanediol		in cosmetics, hydraulic brake fluids (as coupling agent to castor oil) (3)	no data available	
204	lethane	thiocyanic acid 2-(2-butoxyethoxy) ethyl ester		insecticide (3)	moderately irritating to skin and mucous membranes, and, in high conch's narcotic. (3)	Oral LD50 = 91 mg/kg (8)

M/Z	COMPOUND	SYNONYM	STRUCTURE	USES	TOXICITY	TLV
204	pebulate	butyl ethyl thio carbamic acid S-propyl ester		selective herbicide (3)	rapidly metabolised in rats; about 50% of the radio-labelled cpd. administered was expired as CO_2 in 3 days; about 25% in urine and 5% in faeces, (7)	Oral LD50 = 921-1120 mg/kg (8)
208	promecarb	3-methyl-5-(1- methyl ethyl) phenol methyl carbamate		insecticide (3)	chlonisterase inhibitor (3)	
214	salicylanilide			anti-mildew, fungicide (3)	In conc'd form, may cause irritation of skin, mucous membranes. (3)	
219	sulfosalicylic acid	3-carboxy-4-hydroxybenzene sulfonic acid		as metal chelating agents intermediate in the manufacture of surface active agents, organic catalysts and grease additives (3)	Irritating to skin, mucous membranes. (3)	
221	dichlorvos	phosphoric acid 2,2-dichloro ethenyl dimethyl ester		insecticide (3)	Inhalation may cause nuosis, ache eyes, rhinorrhea. Skin/eye contact may cause, nausea, diarrhea, sweating paralysis, low BP, convulsions. (2)	$1 mg/m^3$ (1)
221	purpurogallin	2,3,4,6-tetrahydroxy-5H-benzocy-cylohepten-5-one		as an additive to edible or inedible fats or oils, hydrocarbon fuels or lubricants, retards oxidation or metal contamination (3)	no data available	

M/Z	COMPOUND	SYNONYM	STRUCTURE	USES	TOXICITY	TLV
221	DBMC	2,4-bis (1,1-dimethyl ethyl)-5-methyl phenol		intermediate in the production of rubber chemicals modified phenolic resins (3)	no data available	
221	butylated hydroxy toluene	2,6-bis (1,1- dimethyl-ethyl)-4- methyl phenol		antioxidant for food, animal feed petrol products, synthetic rubbers, plastics, animal and vegatable oils, soaps. Antiskinning agent in paints and inks. (3)	no data available	
221	santalol	5-(2,3-dimethyltricyclo[2.2.1.0] hept-3-yl)-2-methyl-2-penten-1-ol		In perfumes, soaps and detergents (3).	no data available	
222	carbofuran			systemic insecticide, acaricide, nematocide (3)	anti cholinresterase (Reversible). Low to highly toxic. Ing. Inh. or dermal absorbtion may cause constriction of pupils, salivation, profuse sweating, nausea, vomiting, diarrhea (8)	Oral LD50= 8-14 mg/kg (8)
222	bufencarb	3-(1-ethylpropyl) phenol methyl carbamate mixture with 3-(1-methyl butyl) phenyl methyl carbamate mixture with 3-(1-methyl butyl) phenyl methyl carbamate (1:3)	 R= -CH(CH3)(CH2)2CH3 and -CH(C2H5)2	soil and foilage insecticide (3)	Toxic if ingested or absorbed through skin, it inhibits cholinesterase activity in red blood cells (7)	
223	decyl mercaptan derivative		$C_{10}H_{22}SO_3^+$	no data available	no data available	
223	dipentyl sulfide			no data available	no data available	

M/Z	COMPOUND	SYNONYM	STRUCTURE	USES	TOXICITY	TLV
225	cassella's acid	7-hydroxy-2-napthalene sulfonic acid		dyestuff intermediate (3)	no data available	
225	napthol sulfonic acid			preparation of azo dyes (3)	no data available	
225	mevinphos	3-[(dimethoxy phosphinyl) oxy]- 2-butenoic acid methyl ester. Trade name: Phosdrin		contact and systemic insecticide (3)	cholinesterase inhibitor (3)	
226	tinuvin®P.	2-(2H-benzotriazol-2-yl)-4-methyl-phenol		an ultraviolet light absorber for stabilizing plastics and other organic materials against discoloration and deterioration. Effective in protecting polyesters, acrylates, dyes, synthetic and natural fibers, waxes, detergent sol'n, cosmetic formulations (3)	no data available	
240	amino-napthol-sulfonic acid			manuf. of azo dyes (3)	Irritating to eyes, skin, mucous membranes. (3)	

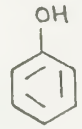
M/Z	COMPOUND	SYNONYM	STRUCTURE	USES	TOXICITY	TLV
240	diphenamid	N,N-dimethyl -α-phenyl benzene acetamide		herbicide (3)	No contact effect to existing plants. Harmful if swallowed (7)	
246	pyrolan	dimethylcarbanic acid 3-methyl-1-phenol-1H-pyrazol-5-yl ester		insecticide (3)	chlolinesterase inhibitor	
235	lenacil	3-cyclohexy-6,7-dihydro -1-H cyclopentapyrimidine-2,4-(3H,5H)-dione		herbicide (3)	no data available	
235	dibenzalacetone	1,5-diphenyl-1,4-pentadien -3-one		in sun protection preparation (3)	no data available	
235	0,0,diethyl-0-(3-methyl-5-pyrazolyl) phosphorothioate			insecticide (3)	cholinesterase inhibitor (3)	
235	quinomethionate	6-methyl-1,3-dithiols [4,5-b]-quinoxalin-2-one		acaricide, fungicide (3)	no data available	

T.L.V. = Threshold Limit Values
P.O.L. = Provisional Operational Limit

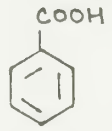
Catalog of chemicals with generic and chemical names and structures, uses and toxicity information.

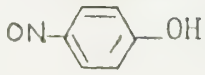
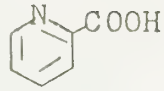
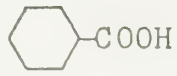
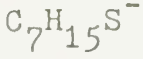
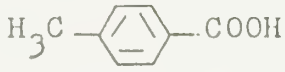
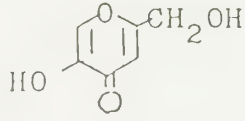
M/Z	COMPOUND	SYNONYM	STRUCTURE	USES	TOXICITY	TLV
45	formic acid		$HC(=O)-OH$	decalcifier, reducer in dyeing wool fast colours, dehairing and plumping hides, tanning, in sizes, electroplating, coagulating rubber latex, also in chemical analysis (3)	dangerously caustic to skin! Chronic absorption has been reported to cause albuminuria, hematuria (3)	5ppm (1)
55	acrolein	2-propenal	$CH_2=CH-CHO$	manuf colloidal forms of metals; making plastics, perfumes; warning agent in methyl chloride refrigerant. Used in organic syntheses. (3) Also used as an aquatic herbicide (7)	irritates skin, mucous membranes. Vapors cause lacrimation. A weak sensitizer; inhalation may cause asthmatic reaction. Inh. of high concns causes pulmonary edema. (3)	0.1ppm (1)
57	thiocyanic acid			no data available	no data available	
59	acetic acid	ethanoic acid		food processing plants; organic chemical mfg; nylon, fiber, dyestuff and pigments mfg; rubber mfg., photographic chemicals & plastics mfg. (3)	Ing may cause severe corrosion of mouth and GI tract, with vomitting, diarrhea, circulatory collapse, eye irritation (3)	10ppm (1)
61	ethylmercaptan		C_2H_5SH	no data available	inhalation causes headache, nausea, muscle irritation, skin or eye contact result in paralysis, pulmonary irritation, liver/ kidney damage (2)	10ppm (2)
69	propiolic acid	2-propynoic acid		no data available	no data available	
71	acrylic acid	2-propenoic acid		in the manuf. of plastics (3)	strong irritant (3)	P.O.L.= 20ppm (5)
72	methyl thiocyanate	methyl sulfocyanate	$CH_3SC\equiv N$	no data available	moderate skin, eye & mucous membrane irritation. Thiocyanate intoxication (6)	none available (6)

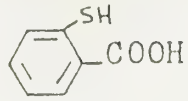
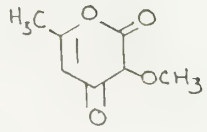
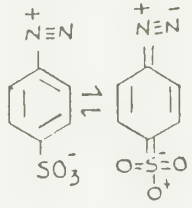
M/Z	COMPOUND	SYNONYM	STRUCTURE	USES	TOXICITY	TLV
73	propanoic acid	propionic acid or methylacetic acid	CH_3CH_2COOH	no data available	liquid causes skin & eye burns. Vapors may irritate eyes, nose & throat, but should not cause systemic illness (6)	toxicity by inhalation: 10ppm (6)
75	thioacetic acid	ethanethioic acid	$CH_3\overset{O}{\overset{\|}{C}}SH$	no data available	no data available	
75	glycolic acid	hydroxy acetic acid	$HOCH_2\overset{O}{\overset{\|}{C}}-OH$	in the processing of textiles, leather and metals; in pH control; in manuf. of adhesives, decontamination cleaning, dyeing (3)	mild irritant to skin and mucous membranes (3)	
77	ethyl sulfonic acid			no data available	no data available	
83	chloric acid		$ClHO_3$	oxidizing agent; with H_2SO_3 as catalyst in acrylonitrile polymerization (3)	strongly irritating to skin and mucous membranes (3)	not available
85	crotonic acid	2-butenoic acid		manuf. of co-polymers with vinyl acetate used in lacquers and paper sizing; in the manuf. of softening agents for synthetic rubber (3)	no data available	
85	methacrylic acid	2-methylpropenoic acid	$CH_2=\overset{CH_3}{\overset{\|}{C}}-COOH$	manuf of methacrylate resins and plastics (3)	may act as a strong irritant. (3)	not pertinent (5)
87	pyruvic acid	2-oxopropanoic acid	$CH_3\overset{O}{\overset{\|}{C}}-COOH$	intermediate in sugar metabolism and in enzymatic carbohydrate degradation where it is converted to acetaldehyde and CO_2 by carbocylase (3)	no data available	
89	lactic acid	2-hydroxy propanoic acid	$HO-\overset{H}{\overset{\|}{C}}-COOH$ (CH3)	occurs in small quantities in blood and muscle fluid of man & animals also present in other organs & body fluids (3)	inhalation of mist causes coughing and irritation of mucous membranes (2)	not available (6)

M/Z	COMPOUND	SYNONYM	STRUCTURE	USES	TOXICITY	TLV
91	propyl mercaptan derivative		$CH_3CH_2CH_2SO^-$	no data available	no data available	not avail. (6)
93	ethyl mercaptan derivative	ethanethiol	$CH_3CH_2SO_2^-$	no data available	no data available	not avail.
93	phenol	hydroxy benzene		as a general disinfectant, either in solution or mixed with slaked lime, etc. for toilets, cesspools, floors, drains, etc. manuf of colorless resins, many medical and industrial organic cpds and dyes; as a reagent for chemical analysis (3)	Chronic poisoning with renal and hepatic damage may occur from industrial contact. Fatal poisoning may also occur by skin absorption. Ingestion of small amts may cause nausea, vomitting, circulatory collapse, paralysis, convulsions, coma, greenish or smoky colored urine and eventually death from respiratory failure (3)	5ppm (1)
95	methanesulfonic acid	methyl sulfonic acid		as catalyst in polymerization, alkylation and esterification reactions, as a solvent (3)	strong irritant (3)	
101	valeric acid	pentanoic acid	C_4H_9COOH	intermediate in perfumery (3)	no data available	not pertinent (5)

M/Z	COMPOUND	SYNONYM	STRUCTURE	USES	TOXICITY	TLV
105	butyl mercaptan derivative		$C_4H_9SO^-$	no data available	no data available	
107	propyl mercaptan derivative		$C_3H_7SO_2^-$	no data available	no data available	
107	cresol			disinfectants and fumigants, in photographic developers; also as a solvent (3)	oral or chronic percutaneous absorption may produce digestive disturbances, nervous disorders with faintness, vertigo, mental changes, skin eruptions, jaundice, general protoplasmic poison (3)	5ppm (5)
108	nicotinyl alcohol	3-pyridine methanol		free alcohol is proposed as a solubilizer for riboflavin (3)	Therap cat: peripheral vasodilator; antilipemic (3)	
111	sorbic acid	2,4-hexadienoic acid		mold and yeast inhibitor. Fungistatic agent for foods, especially cheeses. In alkyd type coatings to improve gloss To improve milling characteristics of cold rubber (3)	no data available	
115	levulinic acid	4-oxopentanoic acid		in organic sythesis; in manuf of nylon, synthetic rubbers, plastics, medicinals (3)	no data available	

M/Z	COMPOUND	SYNONYM	STRUCTURE	USES	TOXICITY	TLV
115	fumaric acid	(E)-butenedioic acid	HOOCCH || HCCOOH	substitute for tartaric acid in beverages and baking powders. As an antioxidant. Manuf polyhydric alcohols, synthetic resins. As mordant in dyeing (3)	Oral ingestion: 500 mg/day for a year is tolerated. Inhalation of dust may cause respiratory irritation (6)	not available (6)
115	maleic acid	(Z)-butenedioic acid		manuf of artificial resins, to retard rancidity of fats and oils; dyeing and finishing wool, cotton and silk (3)	strong irritant to nose, throat, eyes or skin (6)	not available (6)
115	caproic acid	hexanoic acid	$CH_3(CH_2)COOH$	manuf of esters for artifical flavors and of hexyl derivatives, especially hexylphenols, hexylresorcinol etc. (3)	no data available	not pertinent
121	butyl mercaptan derivative		$C_4H_9SO_2^-$	no data available	no data available	
121	ethyl sulfide			no data available	no data available	
121	benzoic acid	benzene carboxylic acid		preserving foods, fats, fruit juices alkaloidal solutions, etc. manuf benzoates and benzoyl cpds, dyes; as a mordant in calico printing, for curing tobacco (3)	Therap Cat: Pharmaceutic aid (antifungal agent) (3) mild irritant to skin, eyes and mucous membranes (6)	not pertinent (6)
121	dimethylphenol			intermediate in mfg of phenolic antioxidants; plastics & resins mfg; disinfectants mfg, insecticides & fungicides, rubber chemicals mfg, wetting agent, dyestuffs (3)	no data available	

M/Z	COMPOUND	SYNONYM	STRUCTURE	USES	TOXICITY	TLV
122	nitrosophenol	quinone oxime		no data available	can cause skin irritation, sensitization (3)	
122	picolinic acid	2-pyridine carboxylic acid		no data available	no data available	
123	propyl mercaptan derivative			no data available		
127	cyclohexane carboxylic acid			solubilizer for vulcanized rubber; clarifier for mineral oil, in insecticide formulations (3)	no data available	
129	heptanoic acid			no data available	no data available	
131	heptyl mercaptan			no data available	no data available	
135	toluic acid	methyl benzoic acid		no data available	no data available	
135	pentyl mercaptan derivative			no data available	no data available	
135	phenylacetic acid			starting material in manuf synthetic perfumes (3)	no data available	
139	fluorobenzoic acid			no data available	no data available	
141	kojic acid	5-hydroxy-2(hydroxy methyl)-4H-pyran-4-one		converted to maltol and ethyl maltol, flavor enhancing additives (3)	no data available	
143	caprylic acid	octanoic acid		an intermediate in manuf of esters used in perfumery; in manuf of dyes, etc. (3)	no data available	

M/Z	COMPOUND	SYNONYM	STRUCTURE	USES	TOXICITY	TLV
153	thiosalicylic acid			manuf of thioindigo dyes (3)		
157	pelargonic acid	nonanoic acid		manuf of lacquers and plastics (3)	strong irritant (3)	
167	dehydroacetic acid	3-acetyl-6-methyl-2H-pyran-2,4(3H)-dione		in organic sythesis; as plasticizer, compatible with nitrocellulose, polystyrene, methacrylate, vinylite resins, (3)	causes impared kidney function, large doses can cause vomitting, ataxia, convulsions (3)	not available
169	dithiosalicylic acid					
171	toluenesulfonic acid	methylbenzene sulfonic acid		in dye chemistry. Also in manuf of oral antidiabetic drugs (3)	highly irritating to skin, mucous membranes	not available (6)
171	capric acid	decanoic acid	$CH_3(CH_2)_8COOH$	manuf of esters for artificial fruit flavors and perfumes; as an intermediate in other chemical synthesis (3)		
183	diazobenzene sulfonic acid			in manuf of azo dyes (3)		
185	iodoacetic acid					

Abbreviations:

T.L.V. = Threshold Limit Values

P.O.L. = Provisional Operational Limit

APPENDIX 4

TAGA CALIBRATION

4.1 GENERAL

The TAGA® calibration, as all other mass spectrometers, consists of two distinct types:

(a) mass calibration

(b) chemical calibration

The mass calibration consists of setting up the analyzer components to obtain accurate molecular weight information and hence empirical structure assignment for the detected peaks. This computer controlled function is done on a daily basis.

The chemical calibration is the injection of known amounts of a particular chemical in order to measure the instrument response and thus correlate the response to the amount of the particular chemical in the sample.

The TAGA® system can be calibrated by injection of known concentrations by:

(a) Direct head space injection.

(b) Flash desorption of low volatility chemicals from a direct insertion probe.

(c) Direct analysis of certified gas mixtures.

The volatile chemicals were calibrated using a silanizied gas tight syringe. A small quantity (less than 0.5 ml) of the liquid was used to coat the inside of the glass syringe. Within a few minutes an equilibrium vapour pressure is achieved within the syringe barrel in a mixture with ambient air. The compound/air mixture is then injected into the TAGA® air inlet stream via an automated syringe drive unit. The concentration of the injected chemical is calculated from the following equation:

$$C\ (ppb) \equiv \frac{P\ (torr)\ Q_S \times 10^9}{760 \times QT}$$

Where -

C (ppb) ≡ the concentration (V/V) of the trace gas in parts per billion (ppb)

P (torr) ≡ the equilibrium vapour pressure of the chemical at the measured temperature

Q_S ≡ the injection rate of the vapour in L/sec from the syringe drive

Q_T ≡ the sampling flow rate (1.4 L/sec) of the TAGA® system

10^9 ≡ is a constant to convert measurements to ppb

760 ≡ is the atmospheric pressure

The calibration of low volatility chemicals was done by the flash desorption of known concentrations deposited on the direct insertion probe.

Using this procedure, the concentration of the trace in the air stream is determined from the following equation:

$$C\ (ppb) \equiv \frac{M_C}{T_D \times Q_T} \times \frac{22.45}{MW} \times \frac{T}{273} \times 10^9$$

Where -

C (ppb) ≡ the concentration (V/V) of the trace chemical in the ambient air carrier gas

M_C ≡ the amount of chemical deposited on the tip of the probe (in micrograms).

T_D ≡ the desorption time determined from the peak width at half height

Q_T ≡ The TAGA® flow rate in L/sec

T ≡ the air stream temperaure in K

MW ≡ the molecular weight of the trace chemical

A comparison between the vapour injection and flash desorption methods for the chemicals shows an agreement within ± 20%.

4.2 RESULTS

Calibration plots are included for:

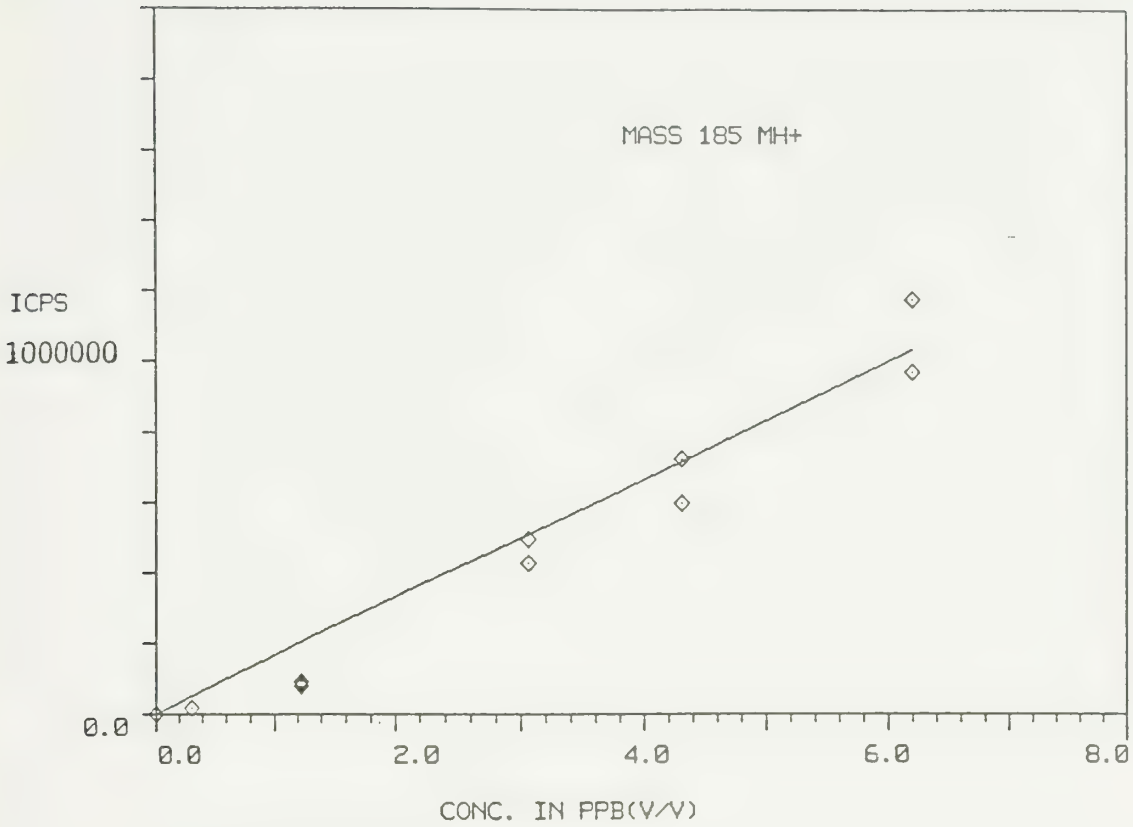
Compound		
benzidine	1.781×10^5	cps/ppb
8-hydroxy quinoline	2.027×10^5	cps/ppb
napthylamine	2.183×10^5	cps/ppb
2,4-xylenol	5.27×10^2	cps/ppb
phenol	6.030×10^3	cps/ppb
n-butylacrylate	1.93×10^2	cps/ppb
acrylic acid	6.76×10^3	cps/ppm
acrolein	1.041×10^4	cps/ppm
aniline	1.357×10^4	cps/ppb
picoline	1.666×10^7	cps/ppm
p-cresol	1.031×10^5	cps/ppb
diphenylamine	1.617×10^5	cps/ppb
maleic anhydride	5.217×10^4	cps/ppb
maleic hydrazide	1.270×10^3	cps/ppb
quinone	2.557×10^5	cps/ppm
sorbic acid	4.336×10^3	cps/ppb
styrene	15.42	cps/ppb
urethane	9.170×10^3	cps/ppb
cyclohexylamine	2.261×10^3	cps/ppb
carbofuran	8.595×10^3	cps/ppb
bufencarb	2.320×10^4	cps/ppb
carbaryl	7.448×10^3	cps/ppb
nitrosodiphenylamine	1.664×10^5	cps/ppb
tri-n-butylamine	8.108×10^3	cps/ppb

The lower detection limits (LDL) for each chemical can be calculated from the calibration constant (Cal. Const.) as follows:

$$LDL = 3\sigma/\text{Cal. Const.}$$

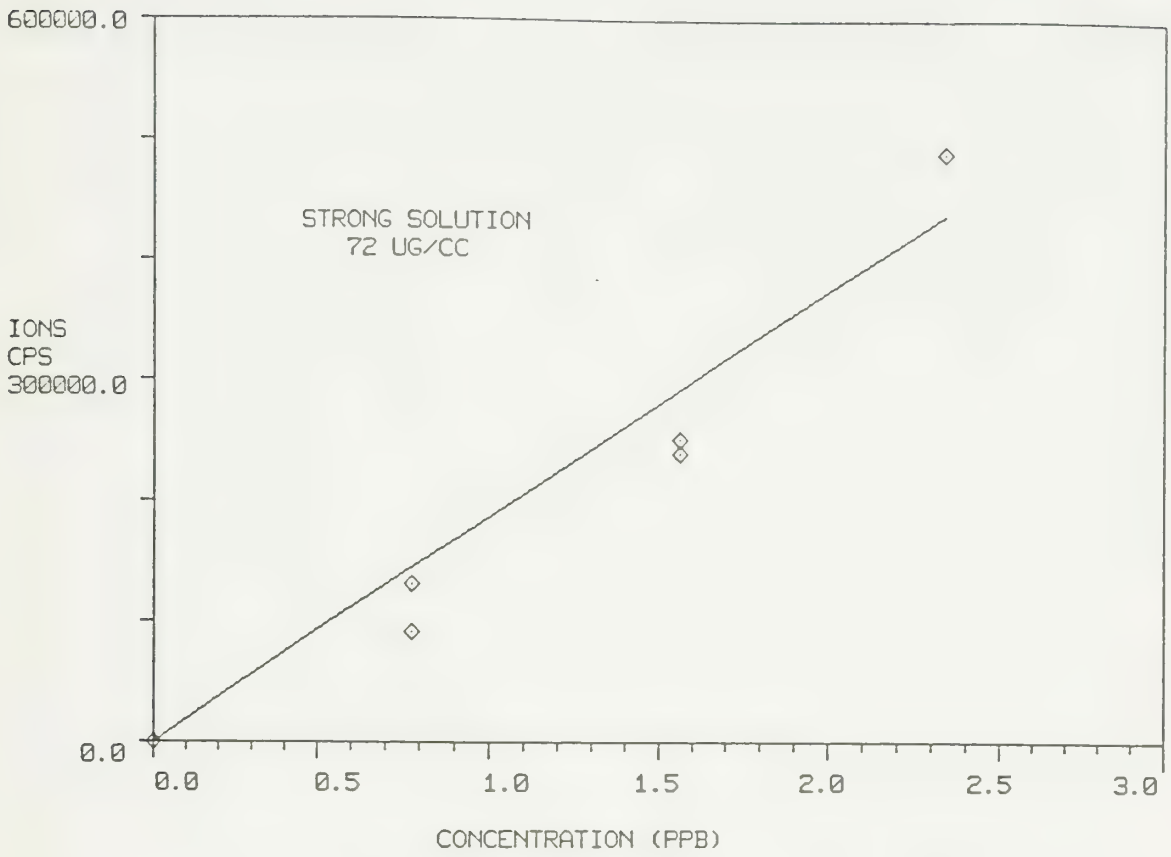
Where σ is the standard deviation of the background signal at the appropriate mass-to-charge. Since the standard deviation of the background is dependent on the ambient air quality, the practical detection limits for each chemical must be measured experimentally for the chemical in its matrix. However, an inherent detection limit (ILDL) can be defined for pure chemicals on the basis of the instrumental electron noise. The standard deviation σ of the electronic noise is 10 cps and hence the ILDL = 30/Cal. Const.

The ILDL for the priority chemicals list names between 0.16 parts-per-trillion (ppt) for benzidine and 2.8 parts-per-billion (ppb) for acrolein.



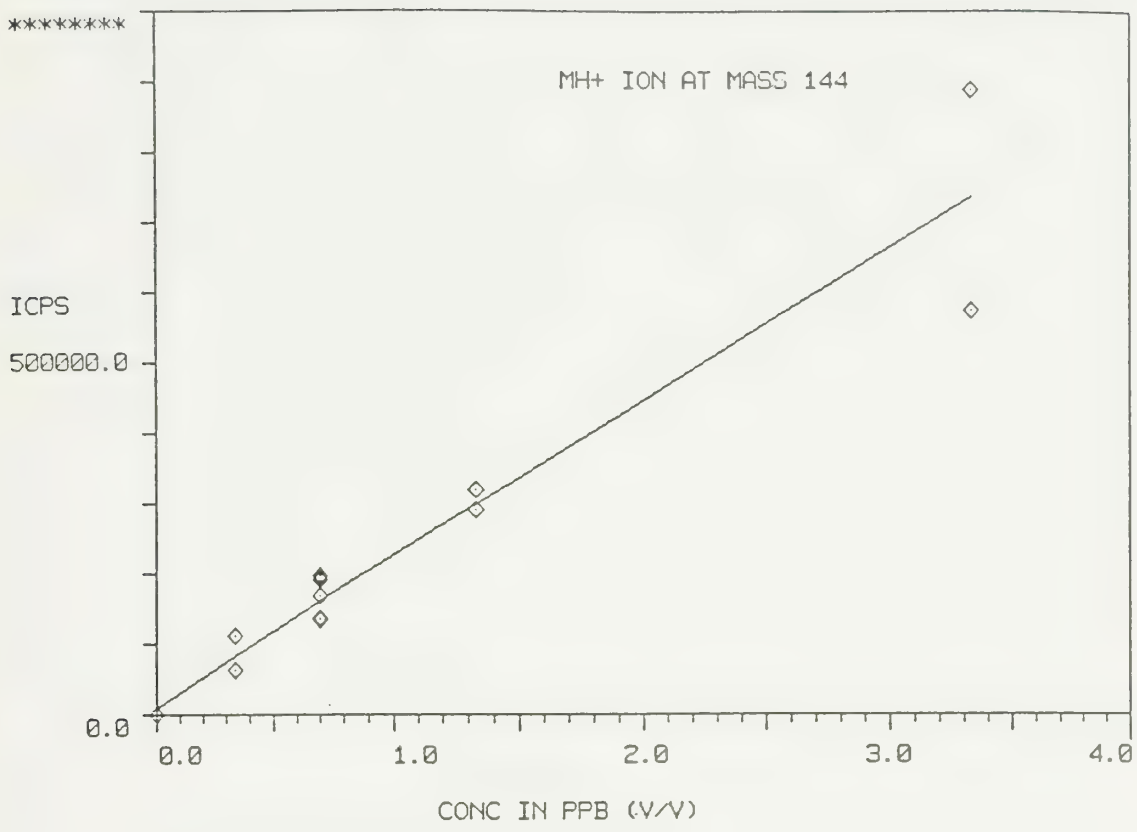
CALIBRATION OF BENZIDINE

FOR DATA SET 1
SLOPE = 0.1781E+06
INTERCEPT = -0.6935E+05
CORR.COE. = 0.984940



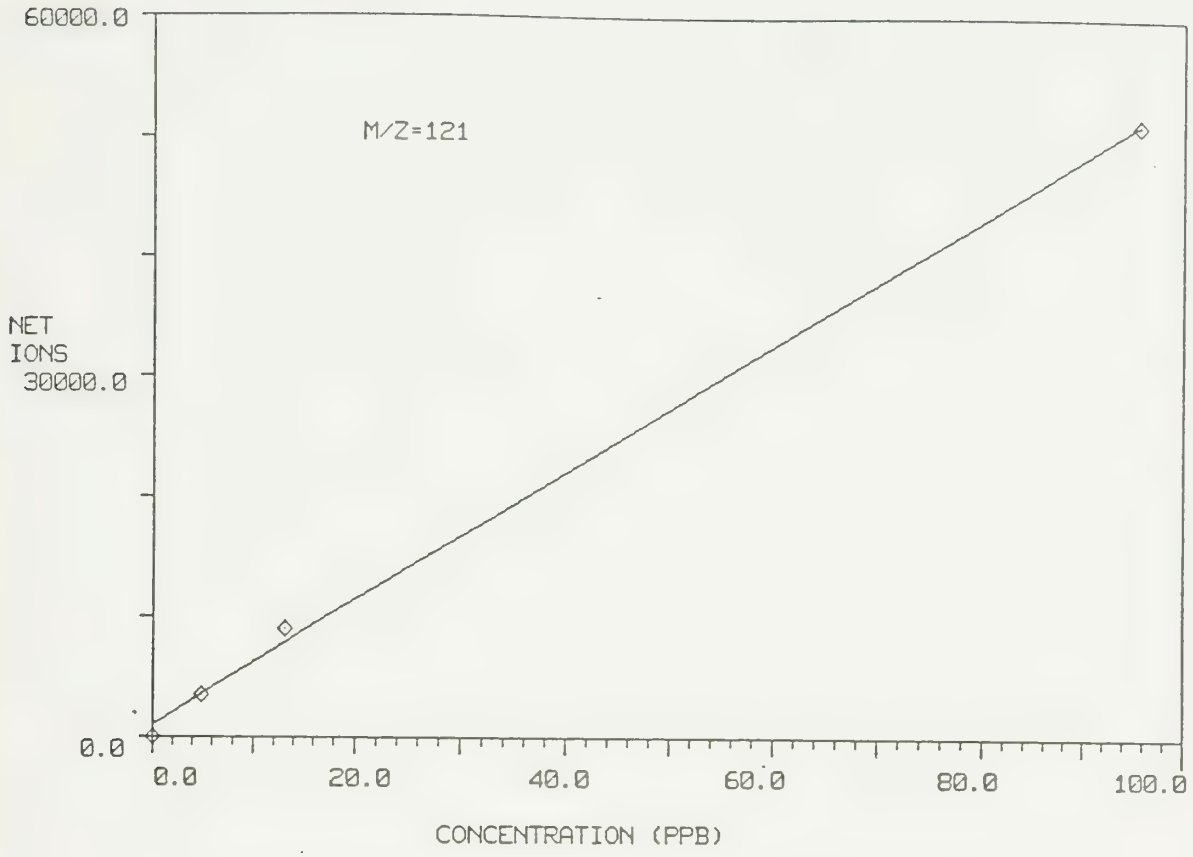
8-HYDROXYQUINOLINE BY FLASH DESORB NET IONS/SEC VS. CONC.

FOR DATA SET 1
SLOPE = 0.2027E+06
INTERCEPT = -0.3602E+05
CORR.COE. = 0.974185



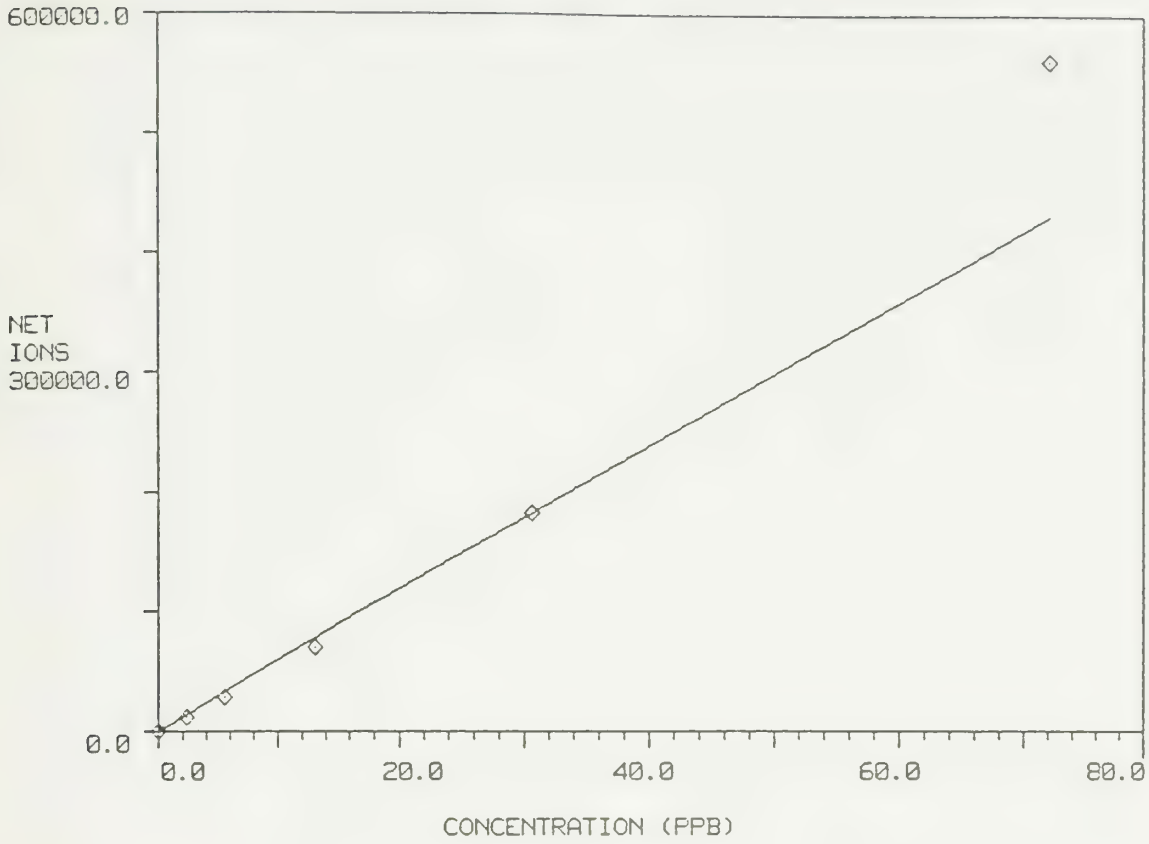
CALIB. OF NAPHTHALAMINE

FOR DATA SET 1
SLOPE = 0.2183E+06
INTERCEPT = 8979.
CORR.COE. = 0.960430



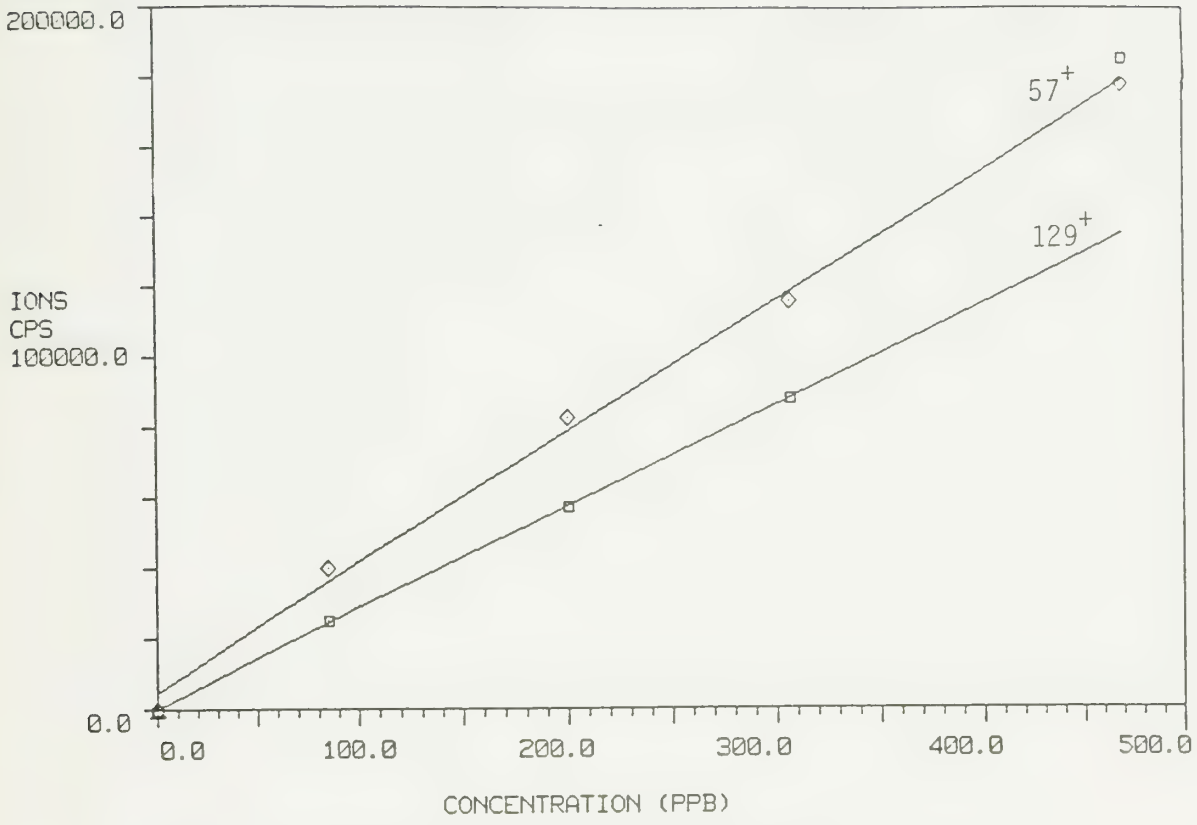
2,4-XYLENOL NET ION COUNTS (COUNTS/SEC) VS. CONCENTRATION

FOR DATA SET 1
SLOPE = 527.3
INTERCEPT = 969.5
CORR.COE. = 0.999366



PHENOL NET ION COUNT (CPS) VS CONCENTRATION (PPB)

FOR DATA SET 1
SLOPE = 6030.
INTERCEPT = -3755.
CORR.COE. = 0.998828



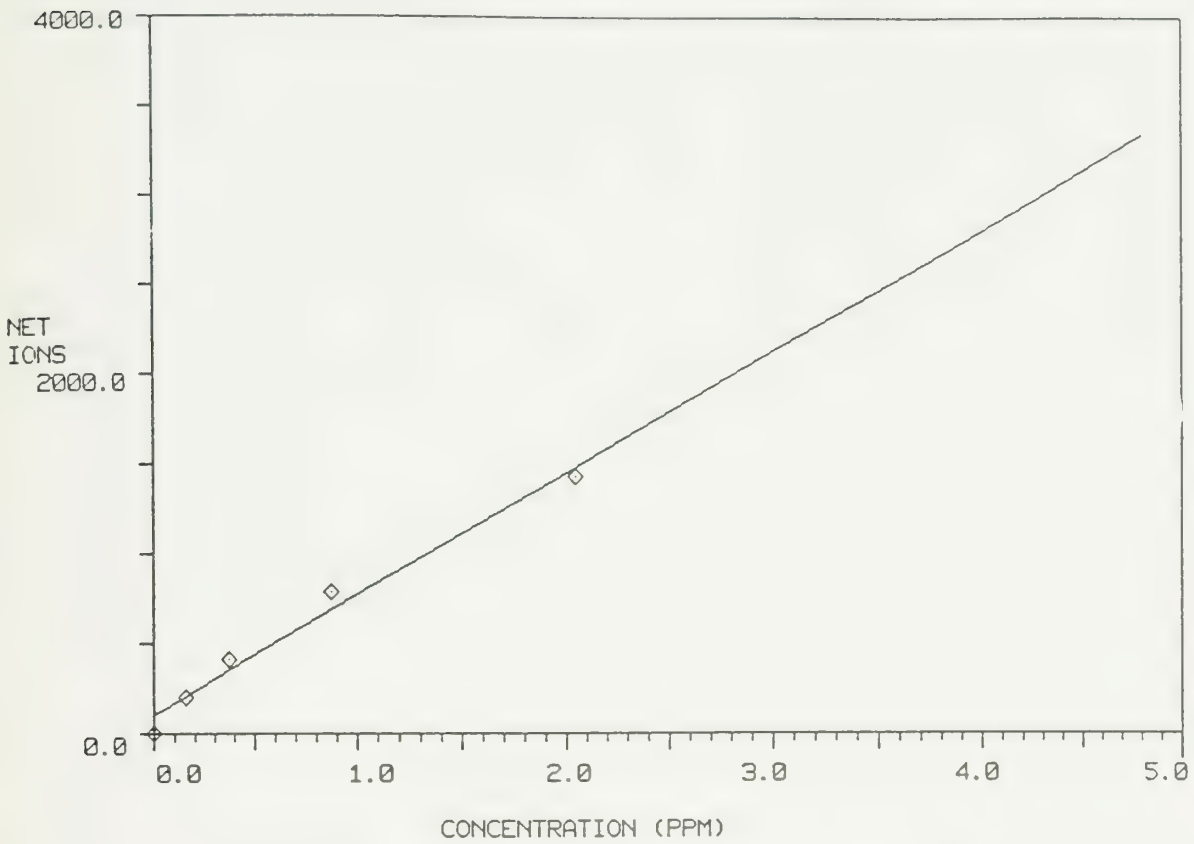
N-BUTYL ACRYLATE NET ION COUNT VS CONCENTRATION

FOR DATA SET 1
SLOPE = 372.4
INTERCEPT = 4512.
CORR.COE. = 0.998475

Mw = 57

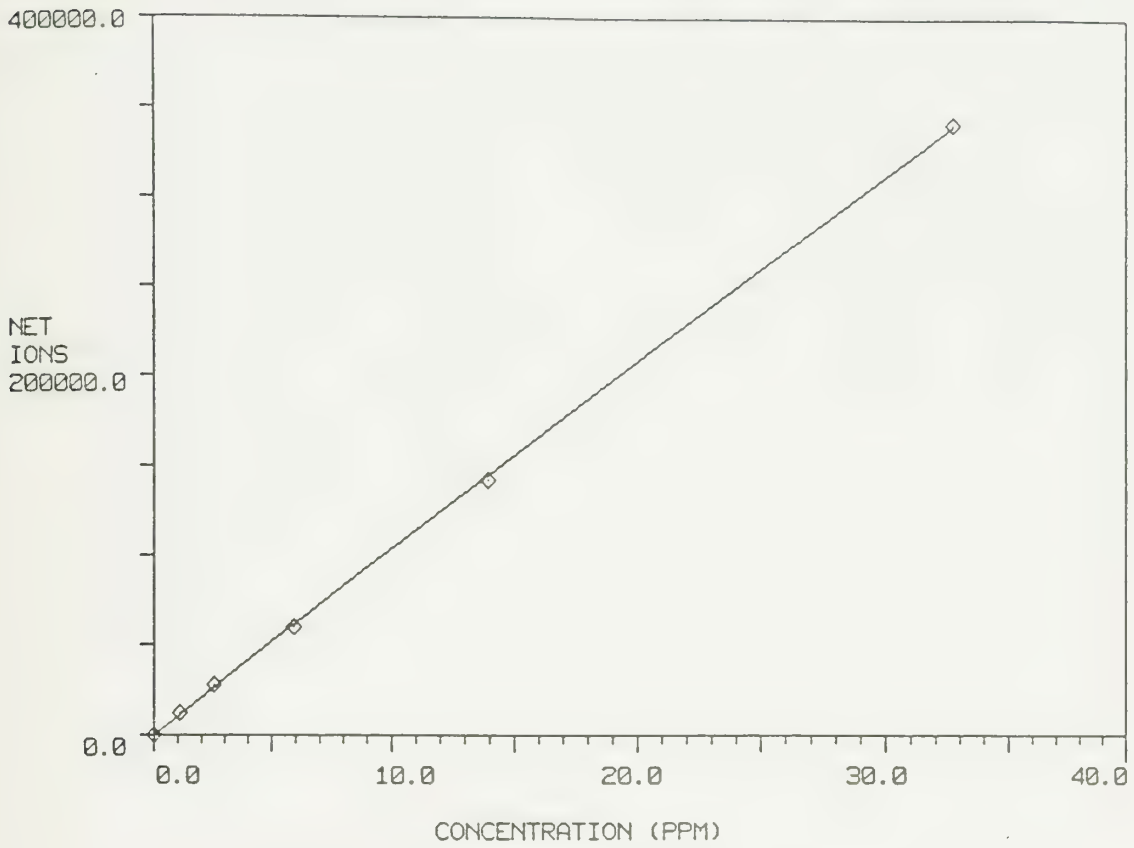
FOR DATA SET 2
SLOPE = 288.3
INTERCEPT = 193.9
CORR.COE. = 0.999987

Mw = 129



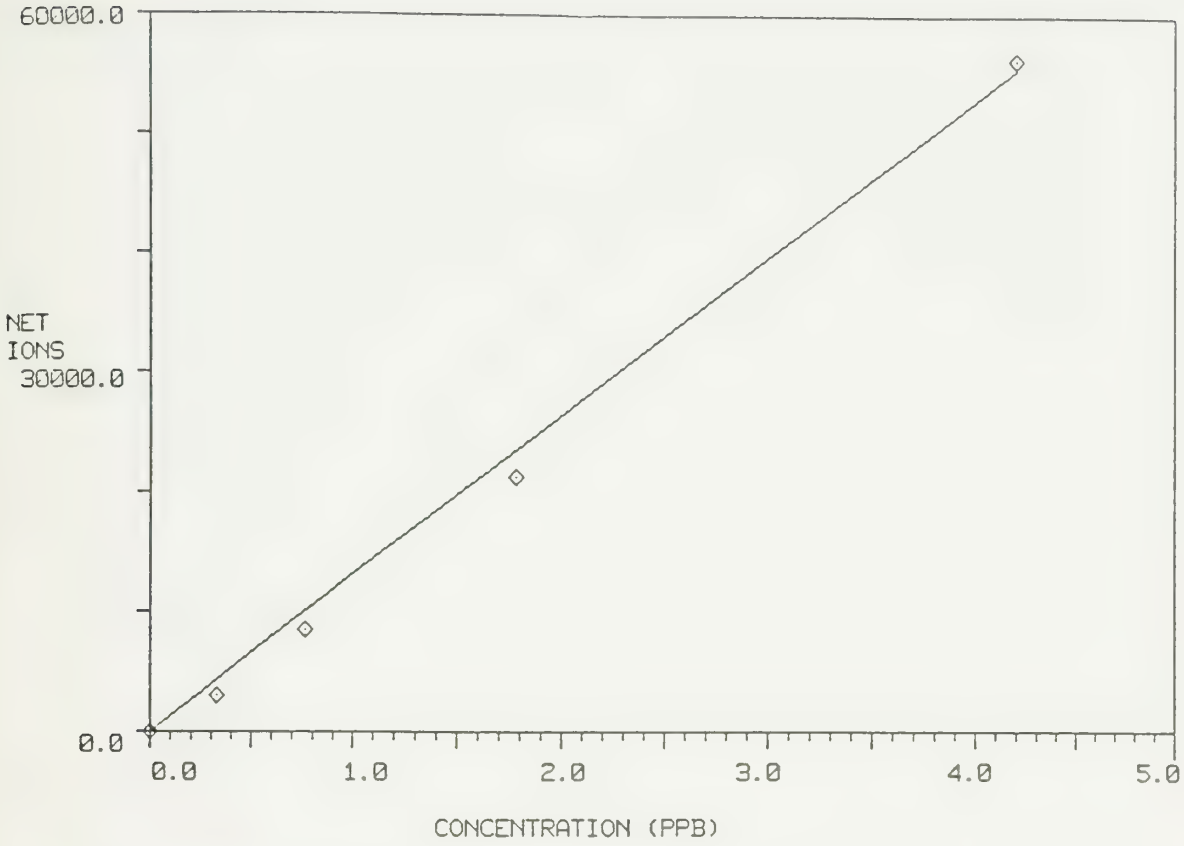
ACRYLIC ACID NET ION COUNT (KILO IONS/SEC) VS CONC. (PPM)

FOR DATA SET 1
SLOPE = 676.2 $\times 10^3$
INTERCEPT = 101.0 K IONS
CORR.COE. = 0.989694



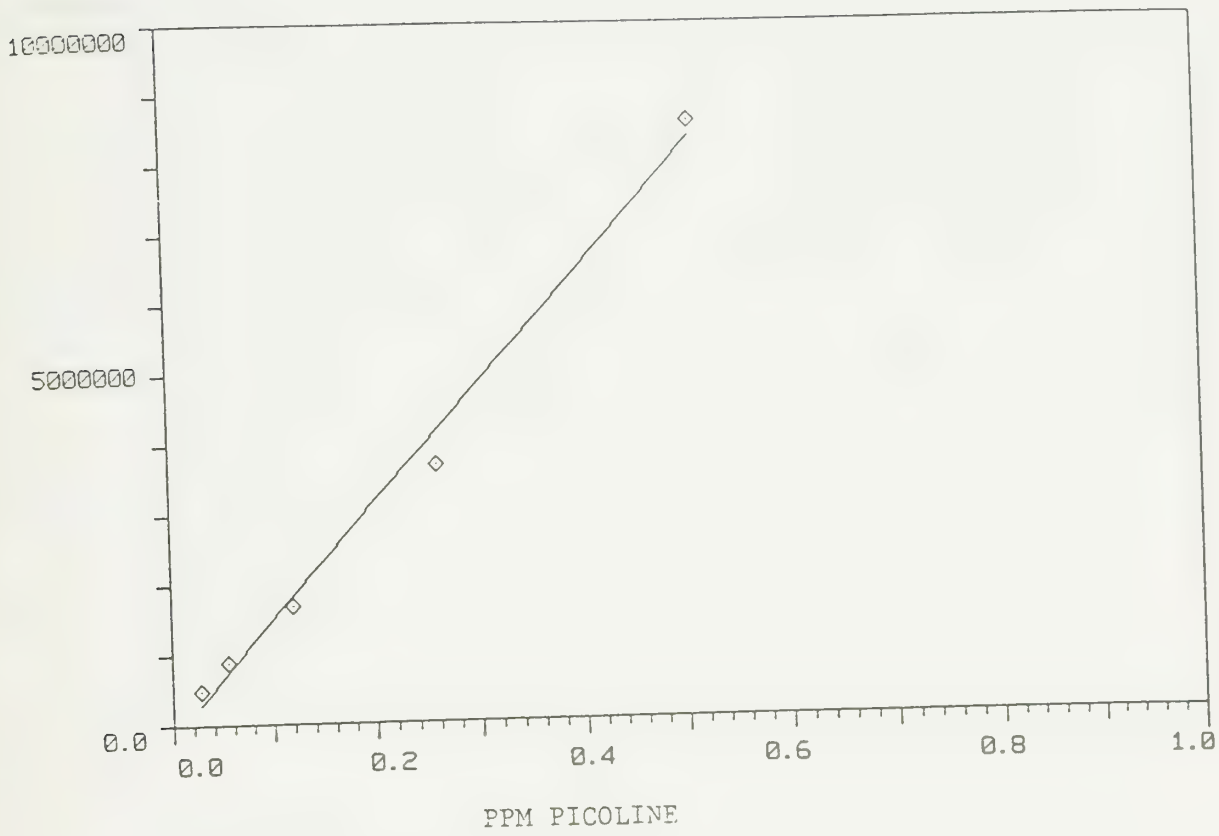
ACROLEIN (2-PROPENAL) NET ION COUNTS VS CONCENTRATION

FOR DATA SET 1
SLOPE = 0.1041E+05
INTERCEPT = -178.5
CORR.COE. = 0.999922



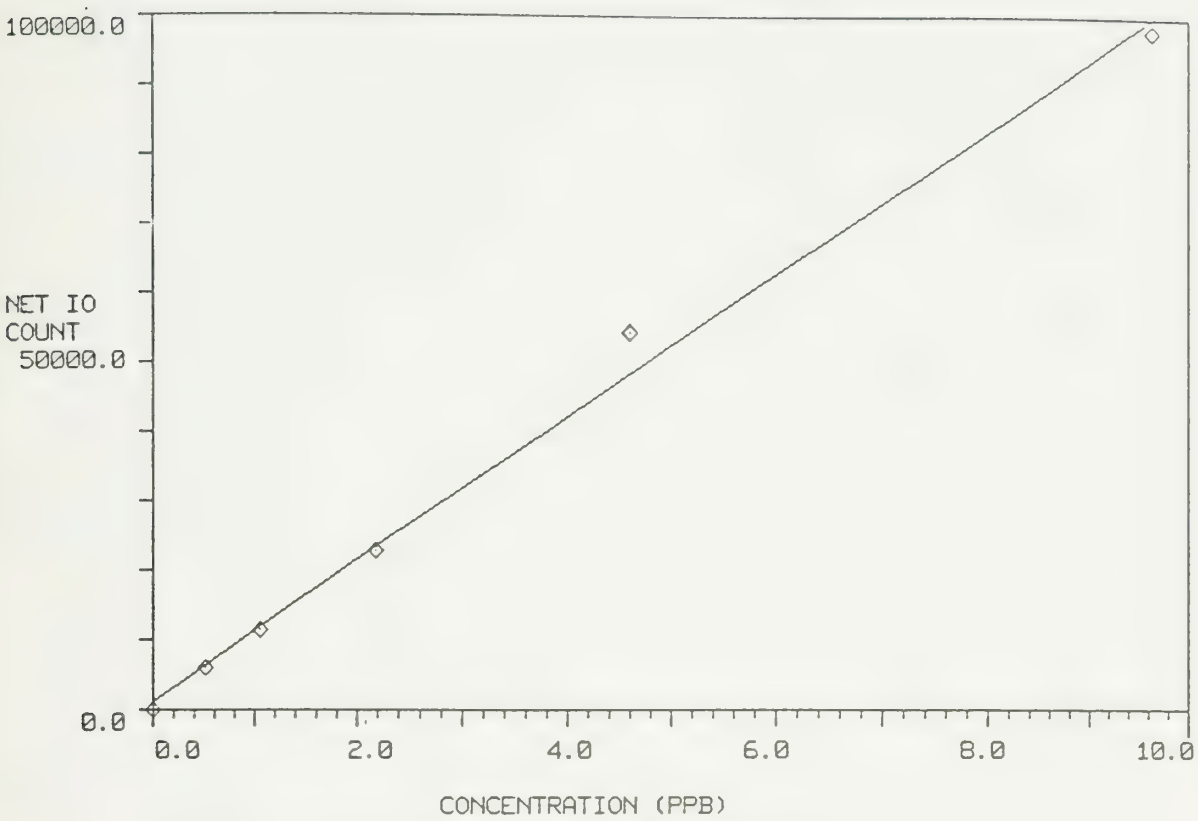
ANILINE NET ION COUNTS (IONS/SEC) VS CONC. (PPB)

FOR DATA SET 1
SLOPE = 0.1357E+05
INTERCEPT = -1343.
CORR.COE. = 0.998731



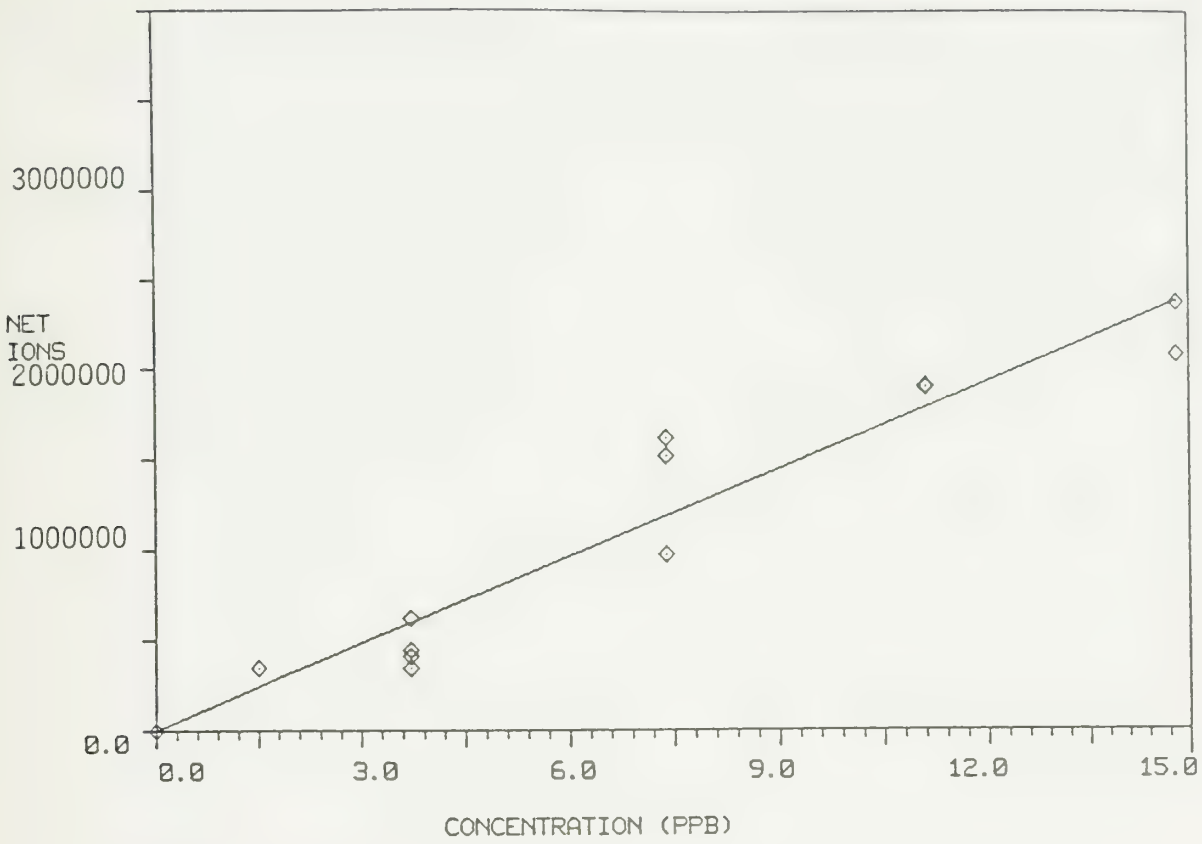
CALIBRATION CURVE FOR PICOLINE

FOR DATA SET 1
SLOPE = 0.1666E+08
INTERCEPT = -0.1603E+06
CORR.COE. = 0.995758



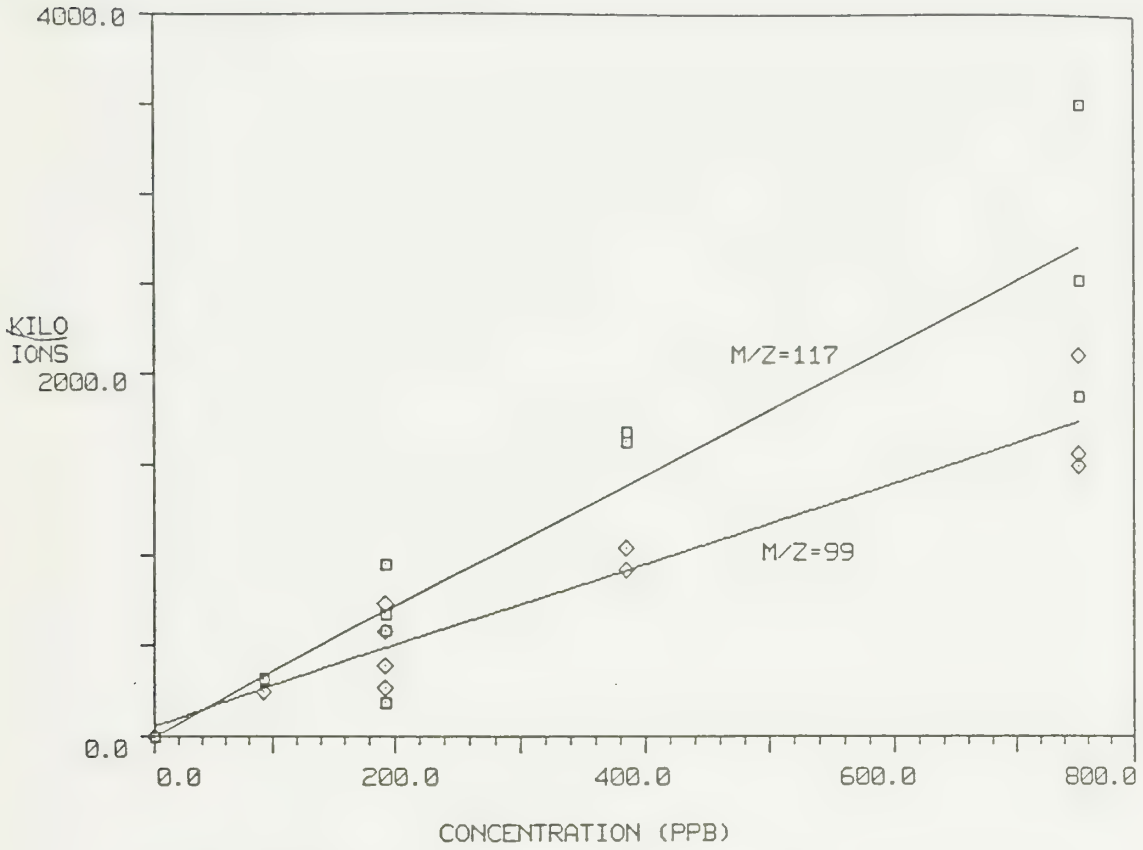
P-CRESOL NET ION COUNT VS CONCENTRATION (PPB)

FOR DATA SET 1
SLOPE = 0.1031E+05
INTERCEPT = 1193.
CORR.COE. = 0.997151



DIPHENYL AMINE STRONG SOLUTION

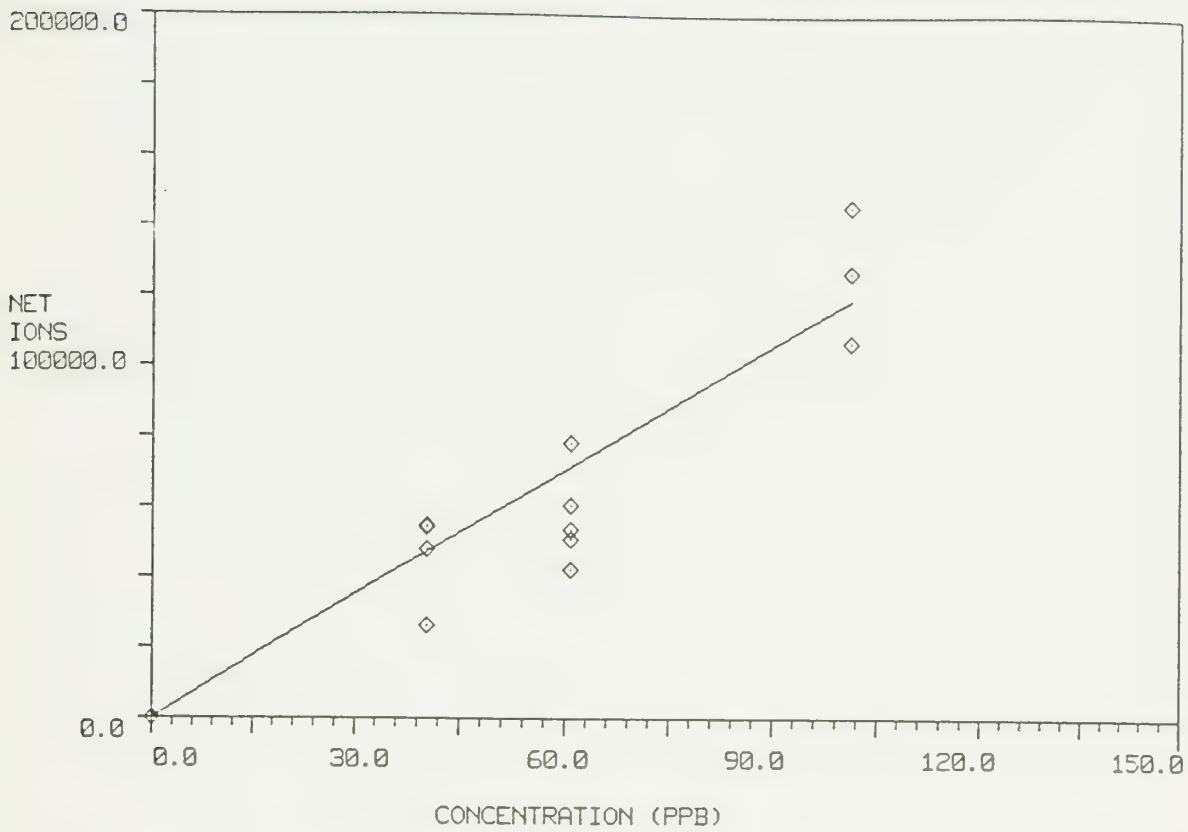
FOR DATA SET 1
SLOPE = 0.1617E+06
INTERCEPT = -2234.
CORR.COE. = 0.962187



MALEIC ANHYDRIDE FLASH DESORB NET IONS/SEC VS. CONCENTRATION

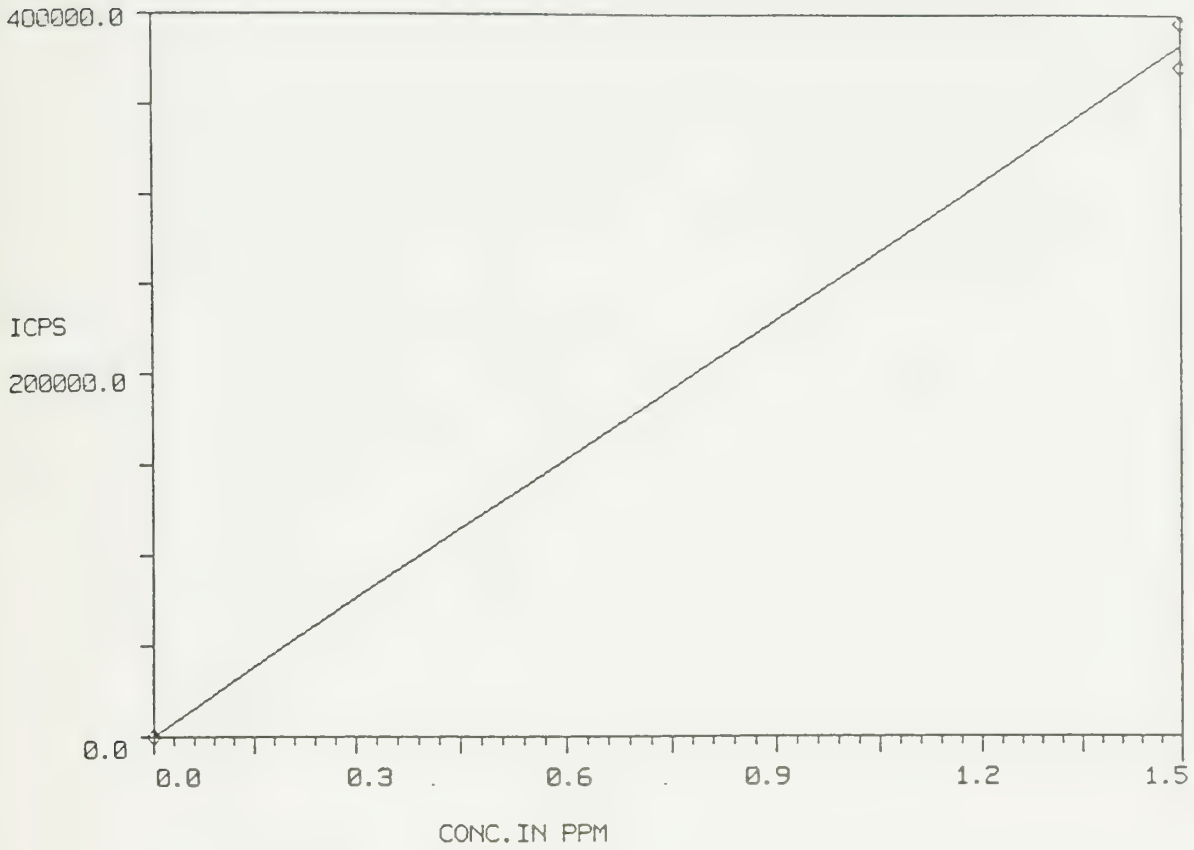
FOR DATA SET 1
SLOPE = 2.254
INTERCEPT = 52.17 x 10^3 m/z = 99
CORR.COE. = 0.958652

FOR DATA SET 2
SLOPE = 3.609
INTERCEPT = -5.456 x 10^3 m/z = 117
CORR.COE. = 0.924885



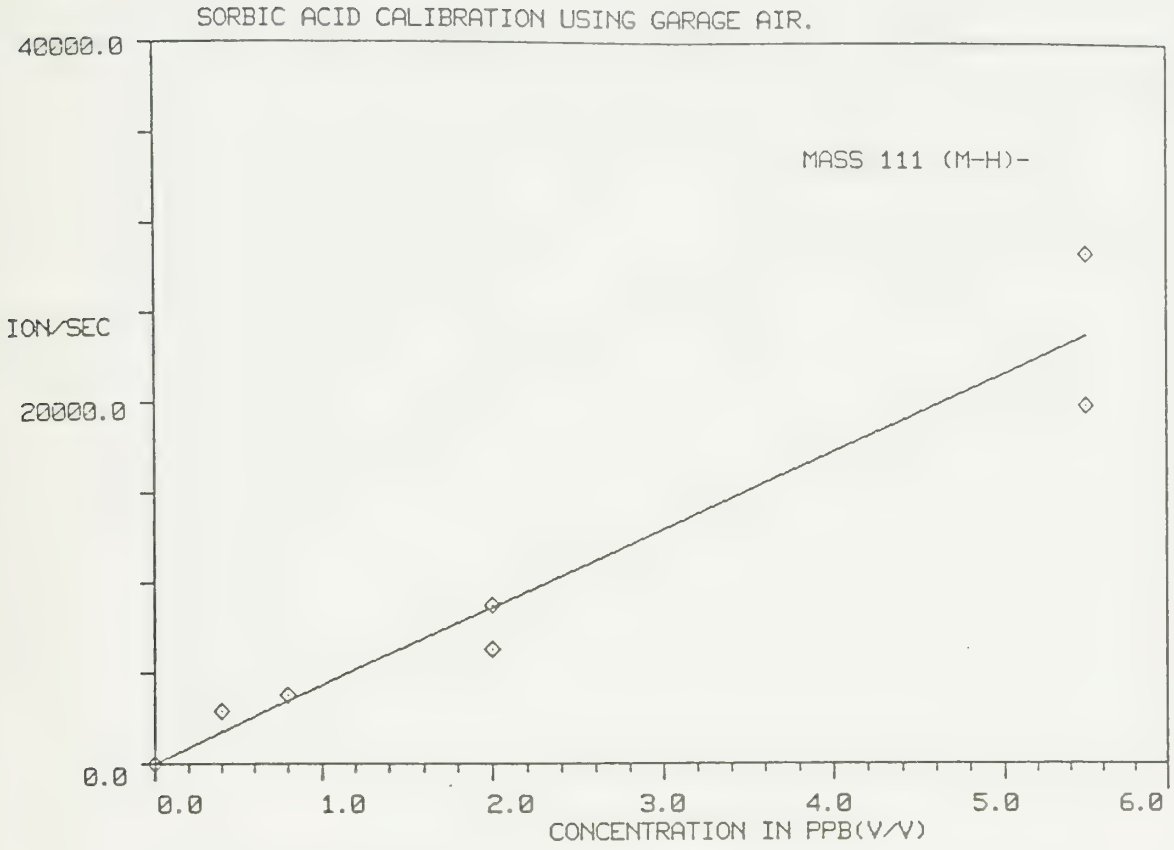
MALEIC HYDRAZIDE CALIBRATION USING FLASH DESORB

FOR DATA SET 1
SLOPE = 1270.
INTERCEPT = -9791.
CORR.COE. = 0.922429

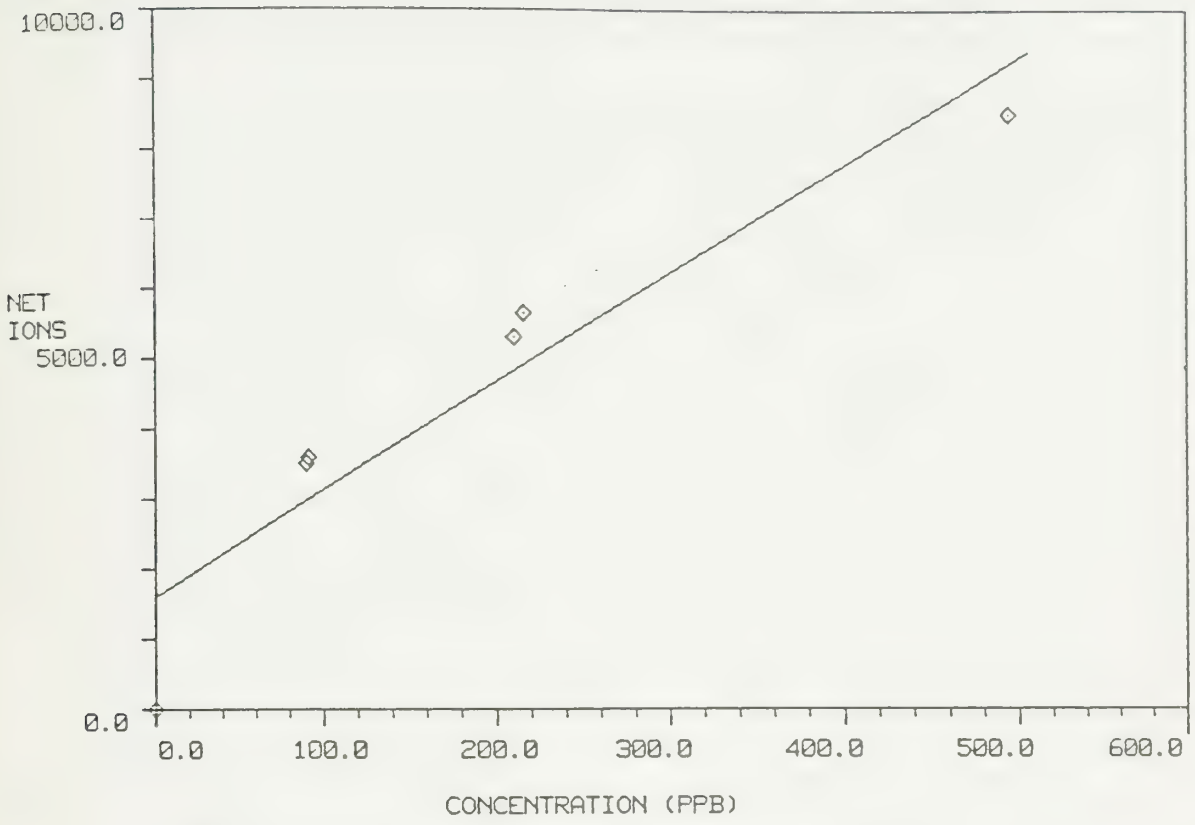


QUINONE CALIBRATION CURVE.

FOR DATA SET 1
SLOPE = 0.2557E+06
INTERCEPT = 0.0000
CORR.COE. = 0.998527

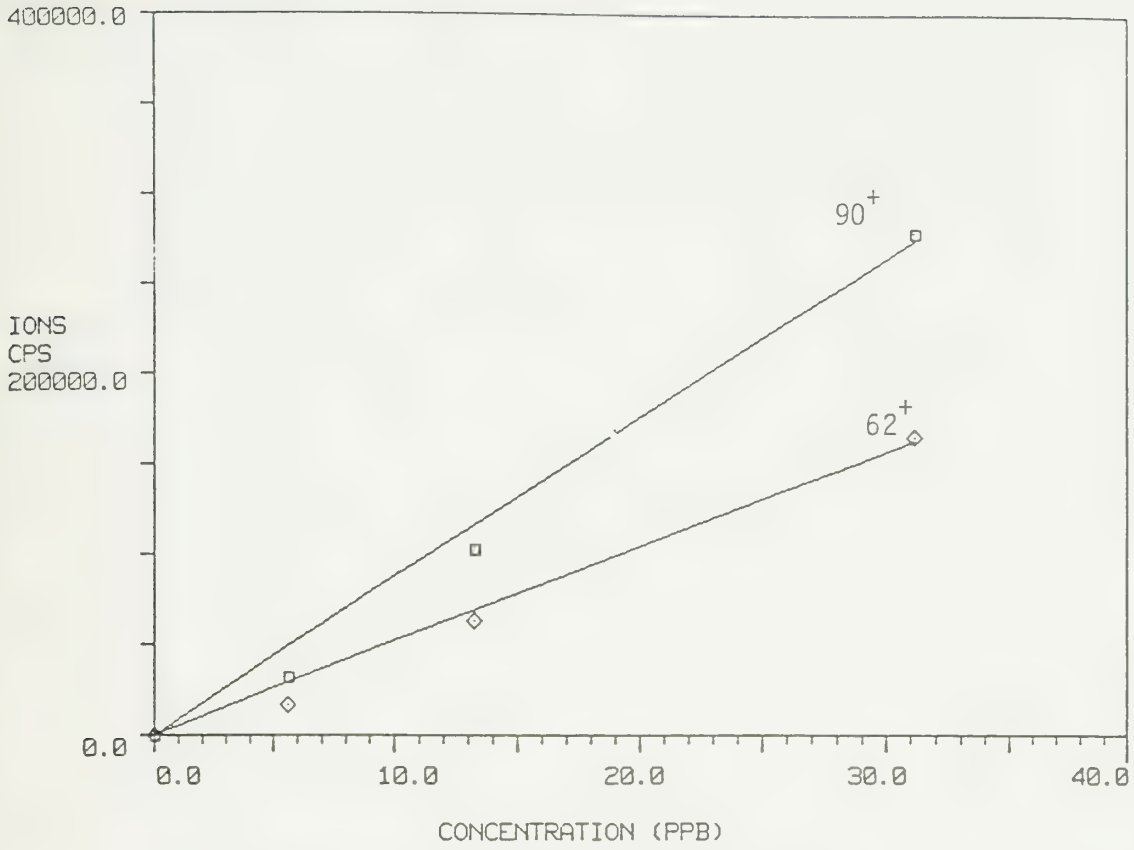


FOR DATA SET 1
SLOPE = 4336.
INTERCEPT = -28.68
CORR.COE. = 0.966333



STYRENE:NET ION COUNTS (COUNTS/SEC) VS. CONC. (PPB)

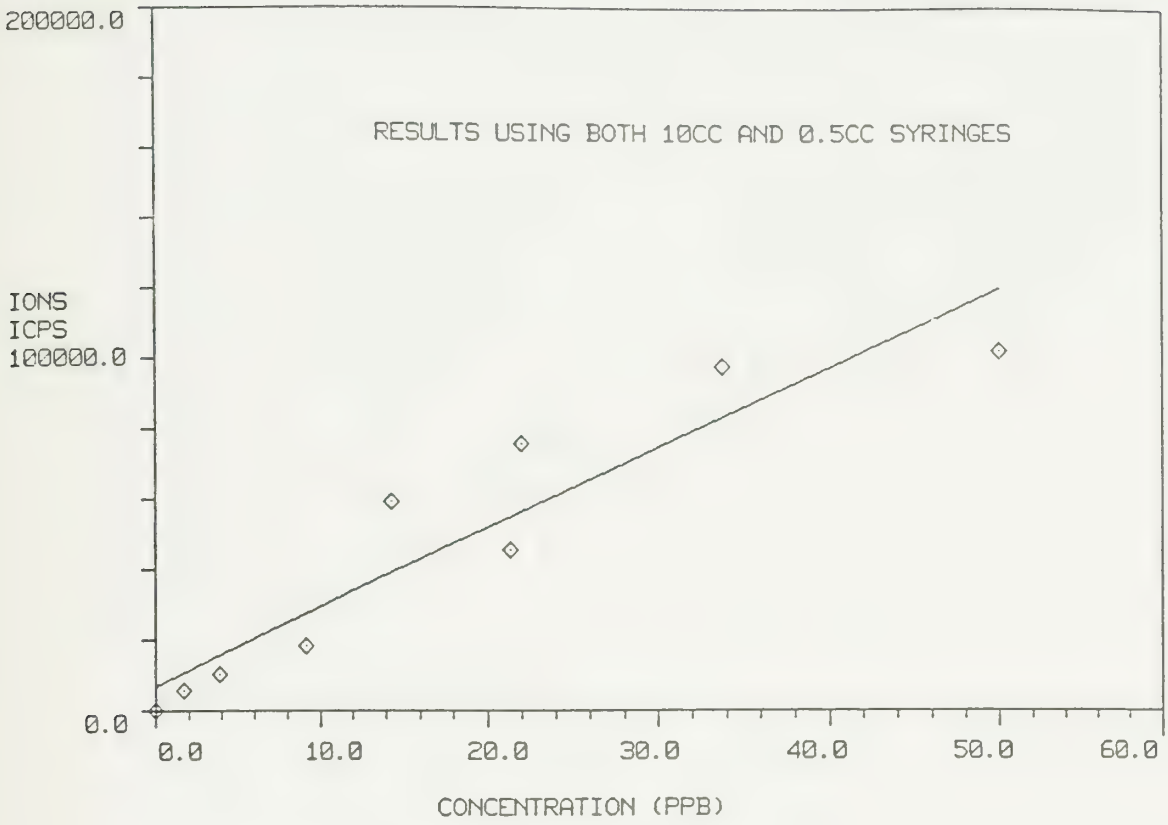
FOR DATA SET 1
SLOPE = 15.42
INTERCEPT = 1595.
CORR.COE. = 0.942765



ETHYL CARBAMATE NET ION COUNTS VS CONCENTRATION

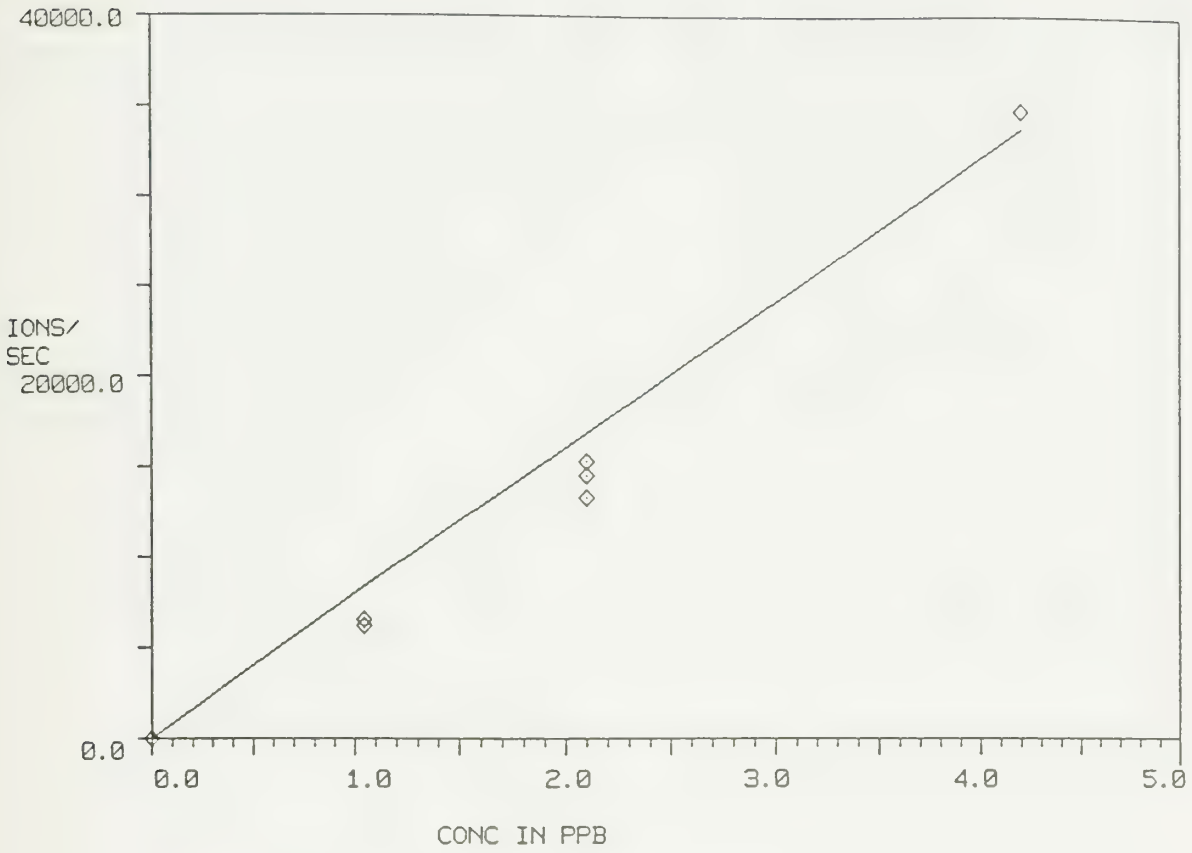
FOR DATA SET 1
SLOPE = 5486.
INTERCEPT = -7189.
CORR.COE. = 0.996623

FOR DATA SET 2
SLOPE = 9170.
INTERCEPT = -0.1038E+05
CORR.COE. = 0.997155



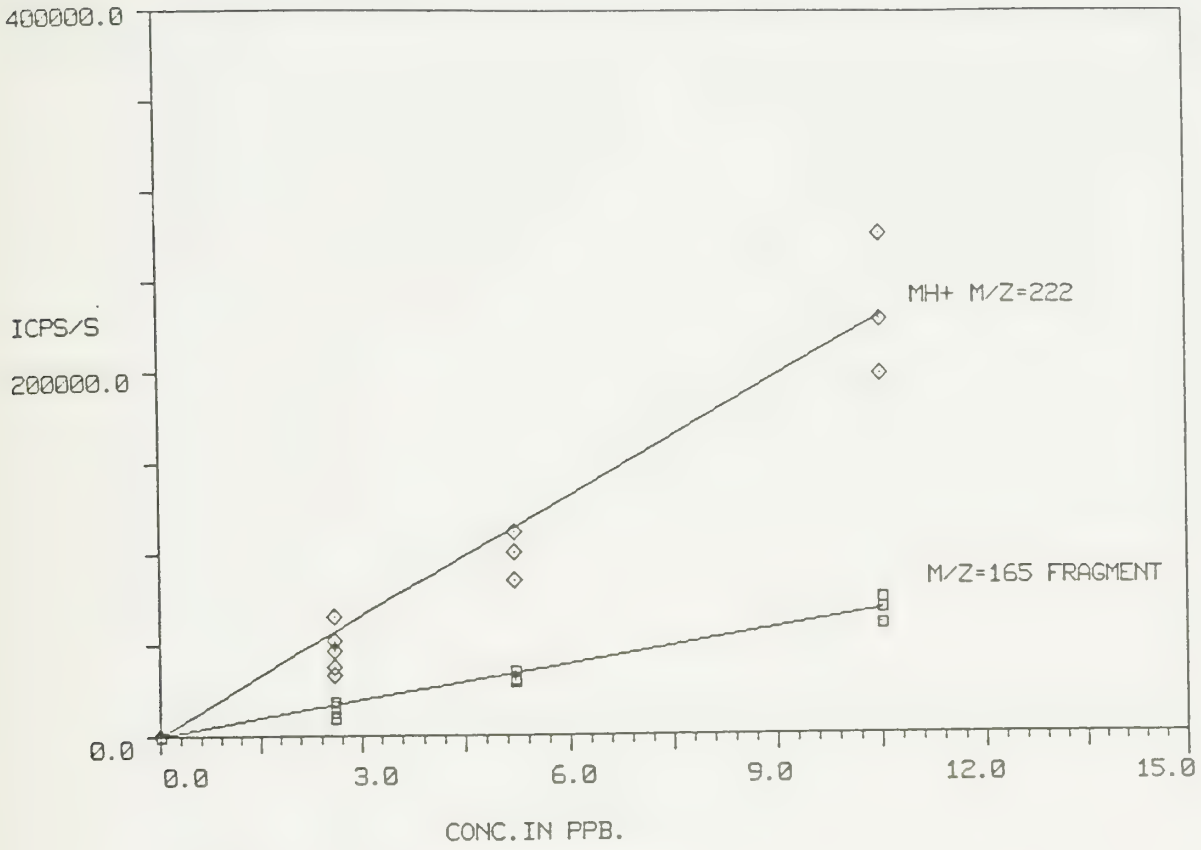
CYCLOHEXYLAMINE CALIBRATION USING SYRINGE DRIVE

FOR DATA SET 1
SLOPE = 2261.
INTERCEPT = 6964.
CORR.COE. = 0.935290



CALIBRATION OF CARBOFURAN USING GARAGE AIR.

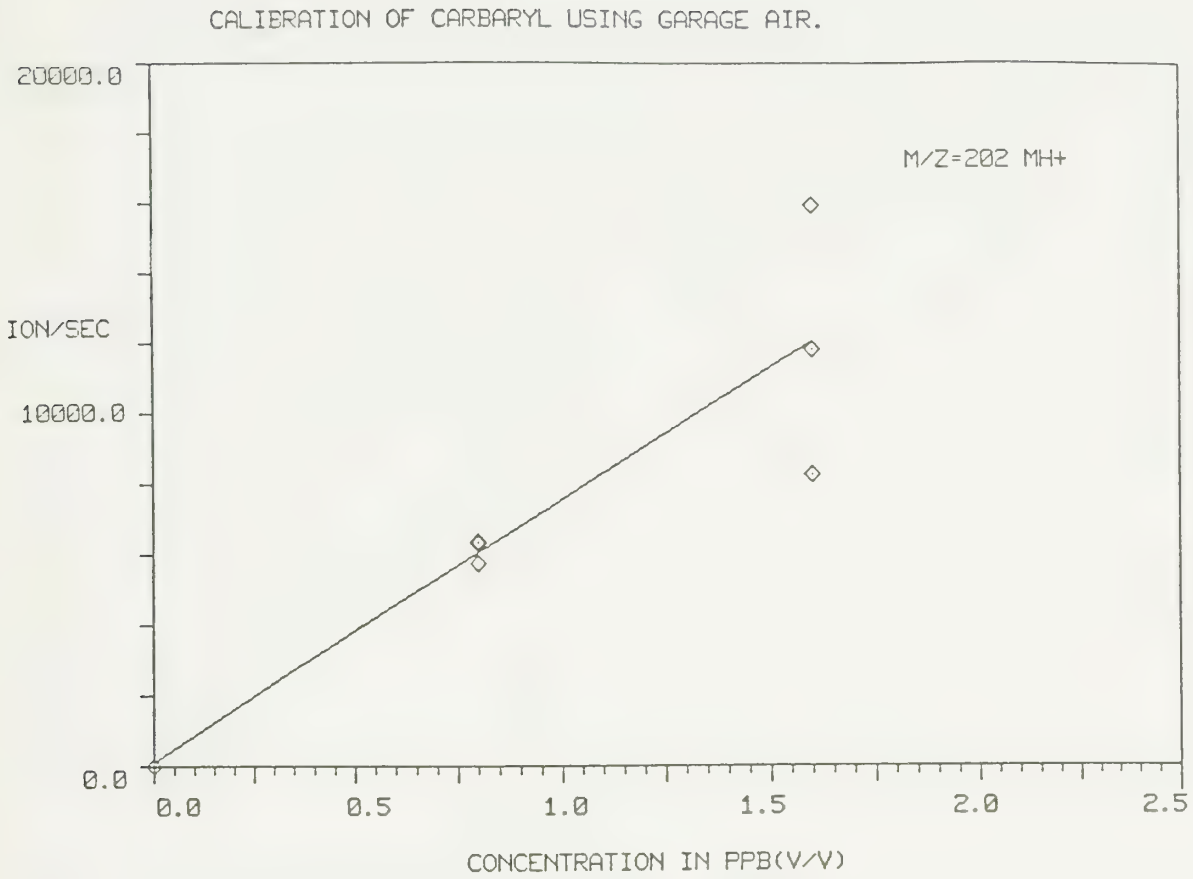
FOR DATA SET 1
SLOPE = 8595.
INTERCEPT = -2345.
CORR.COE. = 0.993454



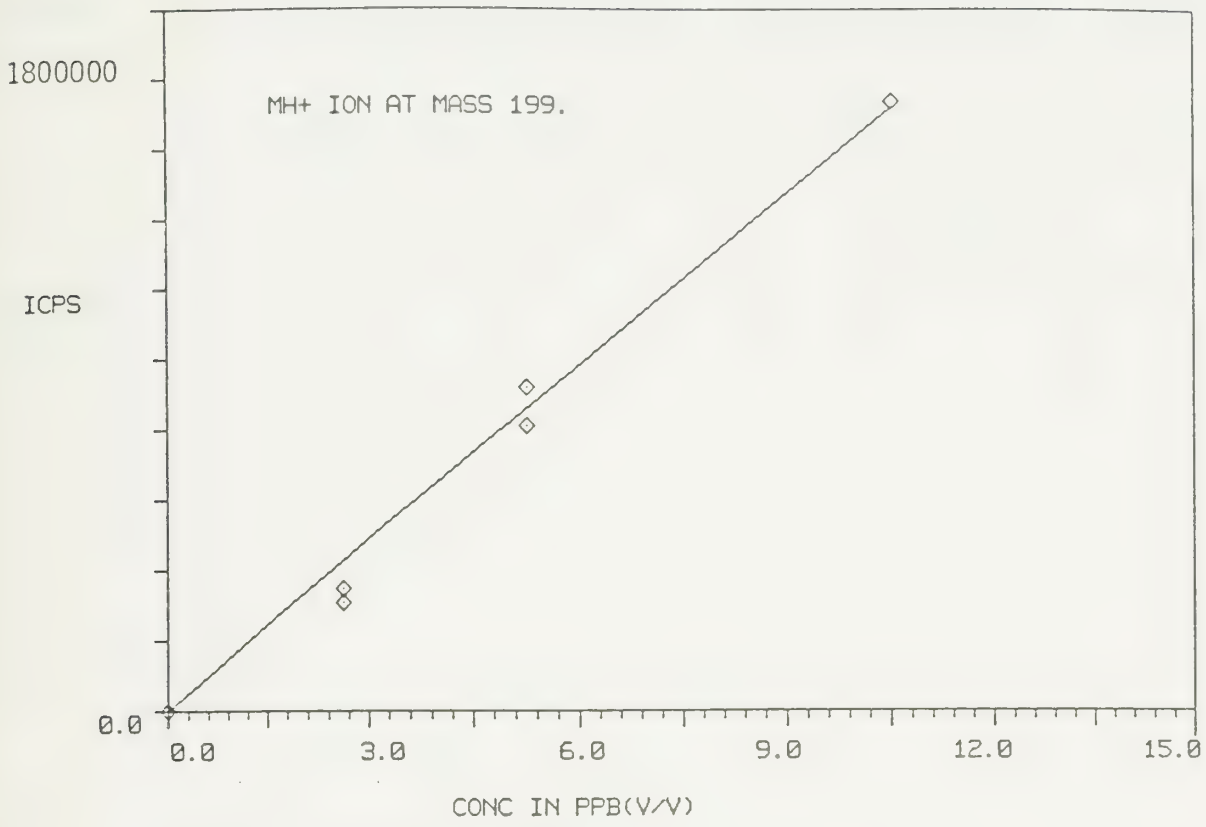
CALIBRATION OF BUFENCARB USING GARAGE AIR.

FOR DATA SET 1
SLOPE = 0.2320E+05
INTERCEPT = -0.1294E+05
CORR.COE. = 0.972681

FOR DATA SET 2
SLOPE = 6799.
INTERCEPT = -2905.
CORR.COE. = 0.985070

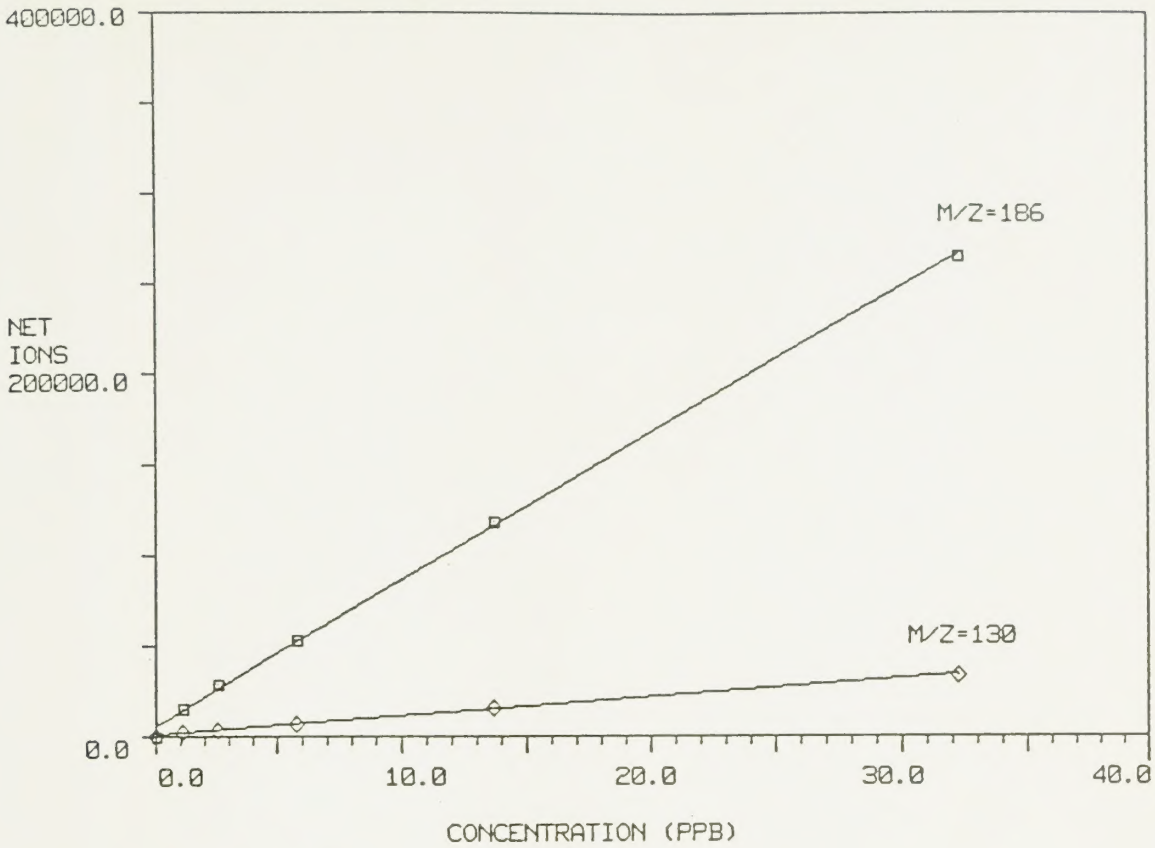


FOR DATA SET 1
SLOPE = 7448.ICPS/PPB
INTERCEPT = 128.4
CORR.COE. = 0.896595



CALIB.OF NITROSODIPHENYLAMINE

FOR DATA SET 1
SLOPE = 0.1664E+06
INTERCEPT = -0.3187E+05
CORR.COE. = 0.995460



TRI-N-BUTYLAMINE CALIBRATION USING SYRINGE

FOR DATA SET 1 M/Z=130
SLOPE = 1036.
INTERCEPT = 699.2
CORR.COE. = 0.999480

FOR DATA SET 2 M/Z=186
SLOPE = 8108.
INTERCEPT = 5577.
CORR.COE. = 0.999491

15 2
8049-20-4

HAMILTON PUBLIC LIBRARY
3 2022 21333778 1